

# Adiabatic evolution of 1D shape resonances: an artificial interface conditions approach.

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## Abstract

Artificial interface conditions parametrized by a complex number  $\theta_0$  are introduced for 1D-Schrödinger operators. When this complex parameter equals the parameter  $\theta \in i\mathbb{R}$  of the complex deformation which unveils the shape resonances, the Hamiltonian becomes dissipative. This makes possible an adiabatic theory for the time evolution of resonant states for arbitrarily large time scales. The effect of the artificial interface conditions on the important stationary quantities involved in quantum transport models is also checked to be as small as wanted, in the polynomial scale  $(h^N)_{N \in \mathbb{N}}$  as  $h \rightarrow 0$ , according to  $\theta_0$ .

## 1 Introduction

The adiabatic evolution of resonances is an old problem which has received various answers in the last twenty years. The most effective results were obtained by remaining on the real spectrum and by considering the evolution of quasi-resonant states (see for example [48][60][1]). Motivated by nonlinear problems coming from the modelling of quantum electronic transport, we reconsider this problem and propose a new approach which rely on a modification of the initial kinetic energy operator  $-\hbar^2\Delta$  into  $-\hbar^2\Delta_{\theta_0}^h$  where  $\theta_0$  parametrizes artificial interface conditions. With this analysis, we aim at developing reduced models for the nonlinear dynamics of transverse quantum transport in resonant tunneling diodes or possibly more complex structures. A functional framework for such a model has been proposed in [45] and implements a dynamically nonlinear version of the Landauer-Büttiker approach based on Mourre's theory and Sigal-Soffer propagation estimates (see [16] and [15] for an alternative presentation of the stationary problem). The derivation of reduced models for the steady state problem has been developed in [20][21][46] on the basis of Helffer-Sjöstrand analysis of resonances in [30]. This asymptotic model elucidated the influence of the geometry of the potential on the feasibility of hysteresis phenomena already studied in [33][50]. Numerical applications have been carried out in realistic  $Ga - As$  or  $Si - SiO_2$  structure in [19] and [18], showing a good agreement with previous numerical simulations in [17] or [41] and finally predicting the possibility of exotic bifurcation diagrams. From the modelling point of view a difficulty comes from the phase-space description of the tunnel effect which can be summarized with the importance in the asymptotic nonlinear system of the asymptotic value of the branching ratio

$$t_j = \lim_{h \rightarrow 0} \frac{|\langle W^h \tilde{\psi}_{-}^h(+k, \cdot), \Phi_j^h \rangle|^2}{4\hbar k \Gamma_j^h}. \quad (1.1)$$

In the above formula  $z_j^h = E_j^h - i\Gamma_j^h$  is a resonance for the Hamiltonian  $H^h = -\hbar^2\Delta + V - W^h$  with a semiclassical island  $V$  and a quantum well  $W^h$ ,  $\tilde{\psi}_{-}(\pm k, \cdot)$  are the generalized eigenfunctions for the filled well Hamiltonian  $\tilde{H}^h = -\hbar^2\Delta + V$  with a momentum  $\pm k$  such that  $k^2 \sim E_j^h$  and  $\Phi_j^h$  is the  $j$ -th eigenfunction of the Dirichlet Hamiltonian  $H_D^h = -\hbar^2\Delta + V - W^h$  on some finite interval  $(a, b)$ . The imaginary part of the resonance is given by the Fermi Golden rule proved in [21]

$$\Gamma_j^h(1 + o(1)) = \frac{|\langle W^h \tilde{\psi}_{-}^h(+k, \cdot), \phi_j^h \rangle|^2}{4\hbar k} + \frac{|\langle W^h \tilde{\psi}_{-}^h(-k, \cdot), \phi_j^h \rangle|^2}{4\hbar k}, \quad (1.2)$$

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where the interaction with the continuous spectrum leading to a resonance contains two contributions from the left-hand side with  $+k$  and from the right-hand side with  $-k$ .

Our purpose is the derivation of reduced models for the dynamics of quantum nonlinear systems like it has been done in the stationary case in [20][21][46] with the following motto: The (nonlinear) phenomena are governed by a finite number of resonant states. As this was already explained in [20], such a remark dictates the scaling of the potential which leads to the small parameter analysis and in the end to effective reduced models even when  $h \sim 0.1$  or  $0.3$  (see [19]).

For the dynamical problem, the time evolution of resonant states have to be considered possibly with a time-dependent potential. And it is known that this is a rather subtle point. Quantum resonances follow almost but not exactly the general intuition (see [53]) and remain an inexhaustible playground for mathematical analysis. For example, the exponential decay law is an approximation which has a physical interpretation in terms of the evolution of quasi-resonant states (truncated resonant states which lie on the real  $L^2$ -space) and writes as

$$e^{-itH^h} \psi_{qr,j} = e^{-itE_j} e^{-t\Gamma_j} \psi_{qr,j} + R(t),$$

where the remainder term  $R(t)$  is small only in the range of times scaled as  $\frac{1}{\Gamma_j}$ . A very accurate analysis of this has been done in [27][57][58][59][39][38] and adiabatic results for slowly varying potentials and for quasi-resonant states have been obtained in [48](see also [60] and [1] in a similar spirit) on this range of time-scales. On the other side the relation

$$e^{-itH^h(\theta)} \psi_j = e^{-itE_j} e^{-t\Gamma_j} \psi_j$$

holds without remainder terms when  $\theta \in i\mathbb{R}_+$  parametrizes a complex deformation of  $H^h$  according to the general approach to resonances (see [3][10][31][23][30][29]). However, and this is well known within the analysis of resonances, the deformed generator  $iH^h(\theta)$  is not maximal accretive although its spectrum lies in  $\{\text{Re } z \geq 0\}$  and no uniform estimates are available on  $e^{-itH^h(\theta)}$ . One of the two next strategies have to be chosen:

- Stay on the real space with quasi-resonant states, with uniform estimates of the semigroups, groups or dynamical systems (they are unitary) but with remainder term which can be neglected only on some parameter dependent range of time.
- Consider the complex deformed situation and try to solve or bypass the defect of accretivity.

Because the remainder terms seemed hard to handle within the original nonlinear problem and also because there may be multiple time scales to handle, due to the nonlinearity or due to several resonances involved in the nonlinear process, we chose the second one.

In a one dimensional problem the simplest approach is the complex dilation method according to [3][10][23]. Since the possibly nonlinear potential with a compact support has a limited regularity inside the interval  $(a, b)$ , this deformation is done only outside this interval following an approach already presented in [54]. The dilation is defined according to

$$U_\theta \psi(x) = \begin{cases} e^{\frac{\theta}{2}} \psi(e^\theta(x-b) + b), & x > b \\ \psi(x), & x \in (a, b) \\ e^{\frac{\theta}{2}} \psi(e^\theta(x-a) + a), & x < a, \end{cases} \quad (1.3)$$

and finally handled with  $\theta \in i\mathbb{R}_+$ . The conjugated Laplacian is

$$U_\theta(-h^2\Delta)U_\theta^{-1} = -h^2 e^{-2\theta \mathbf{1}_{\mathbb{R} \setminus (a,b)}(x)} \Delta,$$

with the domain made of functions  $u \in H^2(\mathbb{R} \setminus \{a, b\})$  with the interface conditions

$$\begin{cases} e^{-\frac{\theta}{2}} u(b^+) = u(b^-); & e^{-\frac{3\theta}{2}} u'(b^+) = u'(b^-) \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+); & e^{-\frac{3\theta}{2}} u'(a^-) = u'(a^+). \end{cases} \quad (1.4)$$

This can be viewed as a singular version of the black-box formalism of [56]. Additionally to the fact that this singular deformation is convenient for the original model with potential barriers presented with a discontinuous potential and with a nonlinear part inside  $(a, b)$ , the obstruction to the accretivity of  $U_\theta(-h^2\Delta)U_\theta^{-1}$  is concentrated in two boundary terms at  $x = a$  and  $x = b$  in

$$\begin{aligned} \operatorname{Re} \langle u, iU_\theta(-h^2\Delta)U_\theta^{-1}u \rangle_{L^2(\mathbb{R})} &= \operatorname{Re} \left[ ih^2(\bar{u}u') \Big|_{a-}^{b+} (e^{-2\theta} - e^{-\frac{\bar{\theta}+3\theta}{2}}) \right] \\ &\quad + h^2 e^{-2\operatorname{Re} \theta} \sin(2\operatorname{Im} \theta) \int_{\mathbb{R} \setminus [a,b]} |u'|^2 dx. \end{aligned} \quad (1.5)$$

Our strategy then relies on the introduction of artificial interface conditions parametrized with  $\theta_0$  which modify the operator  $-h^2\Delta$ . The parameter  $\theta_0$  is then chosen so that the above boundary term vanishes when  $\theta = \theta_0 = i\tau$ . The modified and deformed Hamiltonian  $H_{\theta_0=i\tau}^h(\theta = i\tau)$  then generates a contraction semigroup and uniform estimates are available for  $e^{-itH_{i\tau}(i\tau)}$  or for the dynamical system  $(U^h(t, s))_{t \geq s}$  for time-dependent potentials.

Hopefully this modification has a little effect on the Hamiltonian  $H^h = -h^2\Delta + V - W^h$  and all the quantities involved in the nonlinear problem, with explicit estimates with respect to  $\theta_0$  and  $h$ . Indeed all the quantities and even the exponentially small ones like  $\Gamma_j$  or the ones appearing in the branching ratio (1.1) experiment small relative variation with respect to  $\theta_0$  when  $\theta_0 = ih^{N_0}$  with  $N_0 \geq 5$ .

In comparison with the modelling of artificial dissipative boundary conditions in [11][12][13][14], our approach has the advantage of remaining close to the initial quantum model. Such a comparison is valuable and ensures the validity of numerical applications when the non-linear bifurcation phenomena are very sensitive to small variations of the data.

Once the above comparison is done, it is checked that adiabatic evolution for a slowly varying potential or equivalently for the  $\varepsilon$ -dependent Cauchy problem

$$i\varepsilon \partial_t u = H_{\theta_0}^h(\theta_0, t)u, \quad u_{t=0} = u_0,$$

with some exponentially large time scale  $\frac{1}{\varepsilon} = e^{\frac{c}{h}}$ , is adapted from the general approach for the adiabatic evolution of bound states of self-adjoint generators in [8][43][34].

Adiabatic dynamics have already been considered within the modelling of out-of-equilibrium quantum transport in [22][7][9] playing with the continuous spectrum with self-adjoint techniques. Only partial results are known with non self-adjoint generators: in [42] only small time results are valid for resonances, in [44] bounded generators are considered and in [55] a general scheme for the the higher order construction of the adapted projector is done but without time propagation estimates. In [35], A. Joye considered a general time-adiabatic evolution for semigroups in Banach spaces under a fixed gap condition and with analyticity assumptions: The exponential growth of the dynamical system  $\|S_\varepsilon(t, 0)\| \leq e^{\frac{Ct}{\varepsilon}}$  is compensated by the  $\mathcal{O}(e^{-\frac{c}{\varepsilon}})$  error of the adiabatic approximation under analyticity assumptions (see [43][34]) and lead to a total error  $\mathcal{O}(\frac{Ct-c}{\varepsilon})$  which is small when  $t < c/C$ . Our adaptation combines the uniform estimates due to the accretivity of the modified and deformed Hamiltonian with the accurate resolvent estimate provided by the accurate comparison with self-adjoint problems (shape resonances result from the coupling of some Dirichlet eigenvalues with a continuous spectrum). Although, the error associated with the adiabatic evolution is estimated at the first order as an  $\mathcal{O}(\varepsilon^{1-\delta})$ , with  $\delta > 0$  as small as wanted, it is necessary to reconsider the higher-order method in [43] or [34], because we work with small gaps (vanishing as  $h \rightarrow 0$ ) and with non self-adjoint operators. Finally note that the exponential time scale is not necessarily related with the imaginary parts of resonances and several resonant states with various life-time scales are taken into account in our application.

The outline of the article is the following.

- The artificial interface conditions parametrized by  $\theta_0$  are introduced in Section 2. With these new interface conditions  $-\Delta$  is transformed into a non self-adjoint operator conjugated with  $-\Delta$ ,  $W(\theta_0)(-\Delta)W(\theta_0)^{-1}$  with  $W(\theta_0) = \operatorname{Id}_{L^2} + \mathcal{O}(\theta_0)$ . The case with a potential is illustrated with numerical computations.

- The functional analysis of the complex deformation parametrized with  $\theta$  is done in Section 3. After introducing a Krein formula associated with the  $(\theta_0, \theta)$ -dependent interface conditions, it mimics the standard approach to resonances summarized in [23][29] but things have to be reconsidered for we start from an already non self-adjoint operator when  $\theta_0 \neq 0$ . Assumptions on the time-dependent variations of the potential which ensure the well-posedness of the dynamical systems are specified in the end of this section.
- The small parameter problem modelling quantum wells in a semiclassical island is introduced in Section 4. Accurate exponential decay estimates are presented for the spectral problems reduced to  $(a, b)$  making use of the fact that our operators are proportional to  $-h^2\Delta$  outside  $[a, b]$ .
- The Grushin problem leading to an accurate theory of resonances is presented in Section 5. There it is checked that the imaginary parts of the resonances, which are exponentially small, are little perturbed by the introduction of  $\theta_0$ -dependent artificial conditions. The conclusion of this section is that all the quantities involved in the Fermi Golden Rule (1.2) have little relative variations with respect to  $\theta_0$ , even the exponentially small ones.
- Accurate parameter-dependent resolvent estimates for the whole space problem are done in Section 6. Again the Krein formula for the resolvent associated with the  $(\theta_0, \theta)$ -dependent interface conditions is especially useful.
- The adiabatic evolution of resonances is really introduced in 7. After specifying all the assumptions, the main result about this is stated in Theorem 7.1.
- The appendix contains various preliminary and sometimes well-known estimates, plus a variation of the general adiabatic theory concerned with non self-adjoint maximal accretive operators in Section B

## 2 Artificial interface conditions

Modified Hamiltonians with artificial interface conditions are introduced. It is checked that the effect of these artificial conditions parametrized by  $\theta_0 \in \mathbb{C}$  is of order  $|\theta_0|$  for all the quantities associated with the free Schrödinger Hamiltonian  $-h^2\Delta$  on the whole line. Instead of pursuing this analysis for general Schrödinger operators  $-h^2\Delta + V$  we simply give a numerical evidence of this stability with respect  $\theta_0$ .

### 2.1 The modified Laplacian

We consider a class of singular perturbations of the 1-D Laplacian, defined through non self-adjoint boundary conditions in the extrema of a bounded interval. For  $\theta_0 \in \mathbb{C}$  and  $a, b \in \mathbb{R}$ , with  $a < b$  and  $b - a = L$ , the Hamiltonian  $H_{\theta_0, 0}^h$  is defined by

$$\left\{ \begin{array}{l} D(H_{\theta_0, 0}^h) = \left\{ u \in H^2(\mathbb{R} \setminus \{a, b\}) : \left[ \begin{array}{l} e^{-\frac{\theta_0}{2}} u(b^+) = u(b^-); \quad e^{-\frac{3}{2}\theta_0} u'(b^+) = u'(b^-) \\ e^{-\frac{\theta_0}{2}} u(a^-) = u(a^+); \quad e^{-\frac{3}{2}\theta_0} u'(a^-) = u'(a^+) \end{array} \right] \right\}, \\ H_{\theta_0, 0}^h u = -h^2 \partial_x^2 u, \end{array} \right. \quad (2.1)$$

where  $u(x^+)$  and  $u(x^-)$  respectively denote the right and the left limits of  $u$  in  $x$ , while the notation  $u'$  is used for the first derivative. When  $|\theta_0|$  is small, the analysis of  $H_{\theta_0, 0}^h$  follows by a direct comparison with  $H_{0, 0}^h$  (coinciding with the usual Laplacian:  $-h^2\Delta_{\mathbb{R}}$ ). To fix this point, let us introduce the intertwining operator  $W_{\theta_0}$  defined through the integral kernel

$$W_{\theta_0}(x, y) = \int_{-\infty}^{+\infty} \psi_{-}(k, x) e^{-i\frac{k}{h}y} \frac{dk}{2\pi h}, \quad (2.2)$$

with  $\psi_-(k, x)$  denoting the generalized eigenfunctions associated with our model. These are described by the plane wave solutions to the equation

$$(H_{\theta_0,0}^h - k^2) \psi_-(k, \cdot) = 0. \quad (2.3)$$

For  $k > 0$ , one has

$$1_{(0,+\infty)}(k) \psi_-(k, x) = \begin{cases} e^{i\frac{k}{h}x} + R(k)e^{-i\frac{k}{h}x}, & x < a \\ A(k)e^{i\frac{k}{h}x} + B(k)e^{-i\frac{k}{h}x}, & x \in (a, b) \\ T(k)e^{i\frac{k}{h}x}, & x > b. \end{cases} \quad (2.4)$$

Since  $\psi_-(k, x)$  fulfills the boundary conditions in (2.1), the explicit expression of the coefficients in (2.4) are

$$\begin{cases} A(k) = 2\frac{c_+(\theta_0)e^{-i\frac{k}{h}L}}{d(\theta_0,k)}, & B(k) = -2\frac{c_-(\theta_0)e^{2i\frac{k}{h}a}e^{i\frac{k}{h}L}}{d(\theta_0,k)}, \\ T(k) = \frac{e^{-i\frac{k}{h}L}}{d(\theta_0,k)} (c_+(\theta_0)^2 - c_-(\theta_0)^2), & R(k) = \frac{-2ic_+(\theta_0)c_-(\theta_0)}{d(\theta_0,k)} e^{2i\frac{k}{h}a} \sin\left(\frac{kL}{h}\right), \end{cases} \quad (2.5)$$

with:  $c_+(\theta_0) = e^{\frac{\theta_0}{2}} + e^{\frac{3}{2}\theta_0}$ ,  $c_-(\theta_0) = e^{\frac{\theta_0}{2}} - e^{\frac{3}{2}\theta_0}$  and

$$d(\theta_0, k) = \det \begin{pmatrix} c_+(\theta_0)e^{i\frac{k}{h}a} & c_-(\theta_0)e^{-i\frac{k}{h}a} \\ c_-(\theta_0)e^{i\frac{k}{h}b} & c_+(\theta_0)e^{-i\frac{k}{h}b} \end{pmatrix} = c_+(\theta_0)^2 e^{-i\frac{k}{h}L} - c_-(\theta_0)^2 e^{i\frac{k}{h}L}. \quad (2.6)$$

For  $k < 0$ , an analogous computation gives

$$1_{(-\infty,0)}(k) \psi_-(k, x) = \begin{cases} \tilde{T}(k)e^{i\frac{k}{h}x}, & x < a \\ \tilde{A}(k)e^{i\frac{k}{h}x} + \tilde{B}(k)e^{-i\frac{k}{h}x}, & x \in (a, b) \\ e^{i\frac{k}{h}x} + \tilde{R}(k)e^{-i\frac{k}{h}x}, & x > b, \end{cases} \quad (2.7)$$

with

$$\begin{cases} \tilde{A}(k) = A(-k), & \tilde{B}(k) = e^{4i\frac{k}{h}a} e^{2i\frac{k}{h}L} B(-k), \\ \tilde{T}(k) = T(-k), & \tilde{R}(k) = e^{4i\frac{k}{h}a} e^{2i\frac{k}{h}L} R(-k). \end{cases} \quad (2.8)$$

In what follows we adopt the simplified notation

$$A(k, \theta_0) = \begin{cases} A(k), & k \geq 0 \\ \tilde{A}(k), & k < 0, \end{cases} \quad B(k, \theta_0) = \begin{cases} B(k), & k \geq 0 \\ \tilde{B}(k), & k < 0, \end{cases} \quad (2.9)$$

and

$$T(k, \theta_0) = \begin{cases} T(k), & k \geq 0 \\ \tilde{T}(k), & k < 0, \end{cases} \quad R(k, \theta_0) = \begin{cases} R(k), & k \geq 0 \\ \tilde{R}(k), & k < 0. \end{cases} \quad (2.10)$$

**Lemma 2.1.** *The operator  $W_{\theta_0}$  defined by (2.2) verifies the expansion*

$$W_{\theta_0} - Id = \mathcal{O}(|\theta_0|) \quad (2.11)$$

*in operator norm.*

**Proof:** According to (2.4), (2.7) and to the definition (2.2), one can express the integral kernel  $W_{\theta_0}(x, y)$  as follows

$$\begin{aligned} W_{\theta_0}(x, y) = & \int_{-\infty}^{+\infty} e^{i\frac{k}{h}(x-y)} \frac{dk}{2\pi h} \\ & + 1_{(a,b)}(x) \int_{-\infty}^{+\infty} (A(k, \theta_0) - 1) e^{i\frac{k}{h}(x-y)} \frac{dk}{2\pi h} + 1_{(a,b)}(x) \int_{-\infty}^{+\infty} B(k, \theta_0) e^{-i\frac{k}{h}(x+y)} \frac{dk}{2\pi h} \\ & + 1_{(-\infty,a)}(x) \int_{-\infty}^0 (T(k, \theta_0) - 1) e^{i\frac{k}{h}(x-y)} \frac{dk}{2\pi h} + 1_{(b,+\infty)}(x) \int_0^{+\infty} (T(k, \theta_0) - 1) e^{i\frac{k}{h}(x-y)} \frac{dk}{2\pi h} \\ & + 1_{(b,+\infty)}(x) \int_{-\infty}^0 R(k, \theta_0) e^{-i\frac{k}{h}(x+y)} \frac{dk}{2\pi h} + 1_{(-\infty,a)}(x) \int_0^{+\infty} R(k, \theta_0) e^{-i\frac{k}{h}(x+y)} \frac{dk}{2\pi h}. \end{aligned}$$

The previous expression is rewritten in terms of operators:

$$\begin{aligned} W_{\theta_0} - Id &= 1_{(a,b)} \mathcal{F}^{-1} (A(k, \theta_0) - 1) \mathcal{F} + 1_{(a,b)} P \mathcal{F}^{-1} B(k, \theta_0) \mathcal{F} \\ &\quad + 1_{(-\infty, a)} \mathcal{F}^{-1} 1_{(-\infty, 0)} (T(k, \theta_0) - 1) \mathcal{F} + 1_{(b, +\infty)} \mathcal{F}^{-1} 1_{(0, +\infty)} (T(k, \theta_0) - 1) \mathcal{F} \\ &\quad + 1_{(b, +\infty)} P \mathcal{F}^{-1} 1_{(-\infty, 0)} R(k, \theta_0) \mathcal{F} + 1_{(-\infty, a)} P \mathcal{F}^{-1} 1_{(0, +\infty)} R(k, \theta_0) \mathcal{F}, \end{aligned}$$

where  $\mathcal{F}$  denotes the Fourier transform normalized as  $\mathcal{F}u(k) = \int_{\mathbb{R}} u(x) e^{-i\frac{k}{h}x} \frac{dx}{(2\pi h)^{1/2}}$ , and  $P$  denotes the parity operator:  $Pu(x) = u(-x)$ .

Since the operators  $P$ ,  $\mathcal{F}$ ,  $\mathcal{F}^{-1}$  and multiplication by the characteristic function of a set are uniformly bounded with respect to  $\theta_0$ , we get:

$$\|W_{\theta_0} - Id\| \leq C (\|A(k, \theta_0) - 1\|_{L^\infty(\mathbb{R})} + \|B(k, \theta_0)\|_{L^\infty(\mathbb{R})} + \|T(k, \theta_0) - 1\|_{L^\infty(\mathbb{R})} + \|R(k, \theta_0)\|_{L^\infty(\mathbb{R})}).$$

From (2.8), it is enough to estimate for  $k > 0$  the terms at the r.h.s of the inequality above to get the  $L^\infty(\mathbb{R})$  bounds. Moreover, from the definition of the coefficients  $c_-(\theta_0)$ ,  $c_+(\theta_0)$  and  $d(\theta_0, k)$ , we have:

$$c_-(\theta_0) = \mathcal{O}(|\theta_0|), \quad c_+(\theta_0) = 2 + \mathcal{O}(|\theta_0|), \quad d(\theta_0, k) = 4e^{-\frac{ikL}{h}} + \mathcal{O}(|\theta_0|),$$

where the upper bound of  $\mathcal{O}(|\theta_0|)$  holds with a universal constant. The previous equation gives  $|d(\theta_0, k)| \geq 1$  when  $|\theta_0|$  is small enough, and using (2.5), this implies:

$$\begin{aligned} |A(k, \theta_0) - 1| &= \frac{|2c_+(\theta_0)e^{-\frac{ikL}{h}} - d(\theta_0, k)|}{|d(\theta_0, k)|} = \frac{|\mathcal{O}(|\theta_0|)|}{|d(\theta_0, k)|} \leq C|\theta_0|, \\ |T(k, \theta_0) - 1| &= \frac{|e^{-\frac{ikL}{h}} (c_+(\theta_0)^2 - c_-(\theta_0)^2) - d(\theta_0, k)|}{|d(\theta_0, k)|} = \frac{|2c_-(\theta_0)^2 \sin(\frac{kL}{h})|}{|d(\theta_0, k)|} = \frac{|\mathcal{O}(|\theta_0|^2)|}{|d(\theta_0, k)|} \leq C|\theta_0|, \\ |B(k, \theta_0)| &= \frac{|2c_-(\theta_0)|}{|d(\theta_0, k)|} = \frac{|\mathcal{O}(|\theta_0|)|}{|d(\theta_0, k)|} \leq C|\theta_0|, \\ |R(k, \theta_0)| &= \frac{|2c_+(\theta_0)c_-(\theta_0) \sin(\frac{kL}{h})|}{|d(\theta_0, k)|} = \frac{|(2 + \mathcal{O}(|\theta_0|)) \mathcal{O}(|\theta_0|)|}{|d(\theta_0, k)|} \leq C|\theta_0|. \end{aligned}$$

□

According to the result of Lemma 2.1, for  $|\theta_0|$  small enough,  $W_{\theta_0}$  is invertible; in particular one has

$$W_{\theta_0} = 1 + \mathcal{O}(|\theta_0|), \quad W_{\theta_0}^{-1} = 1 + \mathcal{O}(|\theta_0|). \quad (2.12)$$

Then, it follows from the definition (2.2) that  $H_{\theta_0,0}^h$  are  $H_{0,0}^h$  conjugated operators with

$$H_{\theta_0,0}^h = W_{\theta_0} H_{0,0}^h W_{\theta_0}^{-1}. \quad (2.13)$$

This relation allows to discuss the spectral and the dynamical properties related to  $H_{\theta_0,0}^h$  for small values of the parameter  $\theta_0$ .

**Proposition 2.2.** *There exists  $c > 0$  such that: for any  $\theta_0$  with  $|\theta_0| \leq c$ , the following property holds:*

- 1) *The operator  $H_{\theta_0,0}^h$  has only essential spectrum defined by  $\sigma_{ess}(H_{\theta_0,0}^h) = \mathbb{R}_+$ .*
- 2) *The semigroup associated with  $H_{\theta_0,0}^h$  is uniformly bounded in time and the expansion*

$$e^{-itH_{\theta_0,0}^h} = e^{-itH_{0,0}^h} + \mathcal{O}(|\theta_0|) \quad (2.14)$$

*holds uniformly in  $t \in \mathbb{R}$ .*

**Proof:** 1) According to (2.13), one has

$$(H_{\theta_0,0}^h - z)^{-1} = W_{\theta_0} (H_{0,0}^h - z)^{-1} W_{\theta_0}^{-1},$$

with  $W_{\theta_0}, W_{\theta_0}^{-1}$  bounded in  $L^2(\mathbb{R})$ . This implies:  $\sigma(H_{\theta_0,0}^h) = \sigma_{ess}(H_{0,0}^h) = \mathbb{R}_+$ .

2) Since  $H_{\theta_0,0}^h$  are  $H_{0,0}^h$  conjugated by  $W_{\theta_0}$ , we have

$$e^{-itH_{\theta_0,0}^h} W_{\theta_0} = W_{\theta_0} e^{-itH_{0,0}^h}.$$

For  $|\theta_0|$  small, one can use the expansions (2.12) to write

$$e^{-itH_{\theta_0,0}^h} = W_{\theta_0} e^{-itH_{0,0}^h} W_{\theta_0}^{-1} = (1 + \mathcal{O}(|\theta_0|)) e^{-itH_{0,0}^h} (1 + \mathcal{O}(|\theta_0|)).$$

Recalling that  $H_{0,0}^h$  is self-adjoint (it coincides with the usual Laplacian), and  $(e^{-itH_{0,0}^h})_{t \in \mathbb{R}}$  is a unitary group, one has

$$e^{-itH_{\theta_0,0}^h} = e^{-itH_{0,0}^h} + \mathcal{O}(|\theta_0|).$$

□

**Remark 2.3.** It is worthwhile to notice that  $H_{\theta_0,0}^h$  is not self-adjoint (excepting for  $\theta_0 = 0$ ) neither accretive, since

$$\operatorname{Re} \langle u, iH_{\theta_0,0}^h u \rangle = h^2 \operatorname{Im} \left\{ [\bar{u}(a^-)u'(a^-) - \bar{u}(b^+)u'(b^+)] \left(1 - e^{-\frac{3\theta_0 + \bar{\theta}_0}{2}}\right) \right\}, \quad u \in D(H_{\theta_0,0}^h)$$

has not a fixed sign. Thus, it is not possible to use standard arguments to state that  $e^{-itH_{\theta_0,0}^h}$  is a contraction. Nevertheless, for small values of the parameter  $\theta_0$ , the result of Proposition 2.2 allows to control the operator norm of  $e^{-itH_{\theta_0,0}^h}$  uniformly in time, and states that the time evolution generated by  $H_{\theta_0,0}^h$  is close to the one associated with the usual Laplacian  $H_{0,0}^h$ .

Spectral properties of Hamiltonians obtained as singular perturbations of  $H_{\theta_0,0}^h$  can be discussed using standard results in spectral analysis adapted to this non self-adjoint case.

**Lemma 2.4.** Let  $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$ , with  $\mathcal{V}_1 \in L^\infty((a, b))$  and  $\mathcal{V}_2$  a bounded measure supported in  $U \subset \subset (a, b)$ . Then:  $\sigma_{ess}(H_{\theta_0,0}^h + \mathcal{V}) = \sigma_{ess}(H_{\theta_0,0}^h)$ .

**Proof:** The proof follows from the first point of Corollary 3.4 below in the case  $\theta = 0$ . □

## 2.2 Numerical computation of the time propagators for small $|\theta_0|$

This part is devoted to the numerical comparison of the propagators  $e^{-itH_{\theta_0,V}^h}$  and  $e^{-itH_{0,V}^h}$  where  $V$  is a locally supported perturbation of  $H_{\theta_0,0}^h$  with

$$H_{\theta_0,V}^h = H_{\theta_0,0}^h + V, \quad \text{and} \quad V \in L^\infty((a, b)).$$

Using discrete time dependent transparent boundary conditions for the Schrödinger equation, it is possible to compute the propagator  $e^{-itH_{0,V}^h}$  with a Crank-Nicolson scheme, see [25][6][49][5]. To compute the propagator  $e^{-itH_{\theta_0,V}^h}$ , the key point is to integrate the boundary conditions in (2.1) in the resolution in a way which preserves the stability. This is performed by integrating the boundary conditions in the finite difference discretization of the Laplacian at the points  $a$  and  $b$ . To simplify the presentation, we suppose temporarily that the interface conditions occur only at 0. So we want to write a modified discretization of the operator  $\frac{d^2}{dx^2}$  with the condition

$$\begin{cases} e^{-\frac{\theta_0}{2}} u(0^+) = u(0^-) \\ e^{-\frac{3}{2}\theta_0} u'(0^+) = u'(0^-). \end{cases} \quad (2.15)$$

For a given mesh size  $\Delta x$ , we introduce the discretization of  $\mathbb{R}$ :  $x_j = j\Delta x$  with  $j \in \mathbb{Z}$ . For  $j \neq 0$ , the number  $u_j$  will denote the approximation of  $u(x_j)$ , while  $u_0$  will denote the approximation of  $u(0^-)$  and  $u_0^+$  will denote the approximation of  $u(0^+)$ . If the function  $u$  is regular on  $\mathbb{R}^*$ , we can use the usual finite difference approximation

$$\left(\frac{d^2}{dx^2}u\right)_j = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}, \quad (2.16)$$

for  $j \notin \{-1, 0, 1\}$ . Due to the regularity constraint, this approximation is written correctly for  $j = -1$ , and respectively for  $j = 1$ , only when considering the continuous extension of the function from the left, and respectively from the right, which leads to

$$\left(\frac{d^2}{dx^2}u\right)_{-1} = \frac{u_{-2} - 2u_{-1} + u_0}{\Delta x^2}, \quad \left(\frac{d^2}{dx^2}u\right)_1 = \frac{u_0^+ - 2u_1 + u_2}{\Delta x^2}.$$

With the first relation in (2.15), the approximation at  $j = 1$  is

$$\left(\frac{d^2}{dx^2}u\right)_1 = \frac{e^{\frac{\theta_0}{2}}u_0 - 2u_1 + u_2}{\Delta x^2}. \quad (2.17)$$

At  $j = 0$ , due to the possible discontinuity of a function  $u$  verifying (2.15), we define  $u^-$  on  $\mathbb{R}$  as a regular continuation of  $u|_{(-\infty, 0)}$ . More precisely  $u^- \in C^2(\mathbb{R})$  is such that  $u^- = u$  on  $(-\infty, 0)$  and we get the following approximation at  $j = 0$

$$\left(\frac{d^2}{dx^2}u\right)_0 = \frac{u_{-1} - 2u_0 + u_1^-}{\Delta x^2}. \quad (2.18)$$

This method corresponds to the introduction of a fictive point  $u_1^-$  which allows to write the finite difference approximation for  $\frac{d^2}{dx^2}$  and to calculate  $u'(0^-)$  and  $u'(0^+)$  in (2.15) by using the same points of the space grid

$$\begin{cases} e^{-\frac{\theta_0}{2}}u_0^+ = u_0 \\ e^{-\frac{3}{2}\theta_0}(u_1 - u_0^+) = u_1^- - u_0. \end{cases}$$

The resolution of the system above gives:  $u_1^- = (1 - e^{-\theta_0})u_0 + e^{-\frac{3}{2}\theta_0}u_1$  and (2.18) becomes

$$\left(\frac{d^2}{dx^2}u\right)_0 = \frac{u_{-1} - (1 + e^{-\theta_0})u_0 + e^{-\frac{3}{2}\theta_0}u_1}{\Delta x^2}. \quad (2.19)$$

Therefore, from the boundary conditions in (2.1), the scheme to compute the propagator  $e^{-itH_{\theta_0, \nu}^h}$  is obtained by using the modified Laplacian corresponding to the application of (2.17) and (2.19) at  $x = a$  and  $x = b$ . When  $\theta_0$  is small, the equations (2.17) and (2.19) approximate well the usual finite difference equation (2.16), therefore the solution  $e^{-itH_{\theta_0, \nu}^h}$  will be close to the solution  $e^{-itH_{0, \nu}^h}$ , as expected.

After the change of variable  $x' = \frac{x-a}{\ell} - 1$ , where  $\ell = \frac{b-a}{2}$ , the problem for  $e^{-itH_{\theta_0, \nu}^h}$  is the following

$$\begin{cases} i\partial_t u(t, x) = \left[-\frac{h^2}{\ell^2}\partial_x^2 + \tilde{V}(x)\right] u(t, x), & t > 0, x \in \mathbb{R} \setminus \{-1, 1\} \\ e^{\frac{\theta_0}{2}}u(t, -1^+) = u(t, -1^-), \quad e^{\frac{3}{2}\theta_0}\partial_x u(t, -1^+) = \partial_x u(t, -1^-), & t > 0 \\ e^{-\frac{\theta_0}{2}}u(t, 1^+) = u(t, 1^-), \quad e^{-\frac{3}{2}\theta_0}\partial_x u(t, 1^+) = \partial_x u(t, 1^-), & t > 0 \\ u(0, x) = u_I(x), & x \in \mathbb{R}, \end{cases} \quad (2.20)$$

where  $\tilde{V}(x) = V((x+1)\ell + a)$  and  $u_I \in C^\infty(\mathbb{R})$  is the initial data. The resolution will be performed on the bounded interval  $[-5, 5]$  using homogeneous transparent boundary conditions valid when  $\text{supp } u_I \subset \subset (-5, 5)$ .

Set  $\Delta x = \frac{1}{J}$  and consider the uniform grid points  $x_j = j\Delta x$  for  $j \in \{-5J, \dots, 5J\}$ . Then using



(2.17) and (2.19), the Crank-Nicolson scheme for the modified Hamiltonian is obtained from the Crank-Nicolson scheme in [6][25] by replacing the usual discrete Laplacian by the modified discrete Laplacian defined below

$$\Delta_{\theta_0} u_j = \frac{1}{\Delta x^2} \begin{cases} u_{j-1} - (1 + e^{\mp \theta_0}) u_j + e^{\mp \frac{3}{2} \theta_0} u_{j+1}, & \text{if } j = \pm J \\ e^{\pm \frac{\theta_0}{2}} u_{j-1} - 2u_j + u_{j+1}, & \text{if } j = \pm J + 1 \\ u_{j-1} - 2u_j + u_{j+1}, & \text{else.} \end{cases}$$

The discrete transparent boundary conditions at  $x = -5$  and  $x = 5$  are those used for  $e^{-itH_{0,V}^h}$  in [6][25].

For a given time step  $\Delta t$  and for  $\theta_0 = i \operatorname{Im} \theta_0$ , we present some comparison of the numerical solution  $u_{\theta_0}^n$  to the system (2.20), given at time  $t^n = n\Delta t$  by the scheme described above, with the numerical solution  $u^n$  to the reference problem, computed by taking  $\theta_0 = 0$ . In particular, the numerical parameters are the following:  $\ell = 1$ ,  $h = 0.03$ ,  $J = 30$ ,  $\Delta t = 0.8$ , and the comparison is realized with the initial condition equal to the wave packet

$$u_I(x) = \exp \left( -\frac{(x - x_0)^2}{2\sigma^2} + ik(x - x_0) \right),$$

where  $\sigma = 0.2$ ,  $k = \frac{2\pi}{8\Delta x}$  and the center  $x_0$  will be specified in each simulation.

Three simulations were performed corresponding to different values of the potential  $V$  and of the center  $x_0$ . The first test was realized with  $V = 0$  and  $x_0 = -3$ . Although the comparison presented here can be extended to more general potentials, the two other tests were realized in the case where  $V$  is a non trivial barrier potential

$$V = V_0 I_{(a,b)},$$

where  $V_0 = 0.8$ : for this potential one test was realized with an initial condition localized at the left of  $(-1, 1)$  by taking  $x_0 = -3$ , and the second with an initial condition localized in  $(-1, 1)$  by taking  $x_0 = 0$ . The solution  $u_{\theta_0}^n$  is represented, at different time  $t$ , next to the reference solution  $u^n$  in the Figures 1, 2 and 3, for the fixed small value  $\theta_0 = 0.09i$ . We remark that  $u_{\theta_0}^n$  has the same qualitative behaviour than the reference solution.

In the case  $V = 0$ , the solution  $u_{\theta_0}^n$  corresponds to an incoming function from the left which goes near the domain  $(-1, 1)$ . When time grows, it crosses the interface points and leaves the domain.

In the case of the barrier potential with  $x_0 = -3$ , the solution is splitted in two parts: a first one which passes through the barrier; and a second one which is reflected and goes out of the domain.

In the case of the barrier potential with  $x_0 = 0$ , it appears that the wave packet is splitted in two outgoing parts: one which leaves the barrier on the left and the second on the right. The part on the right is more important and goes out faster, it is due to the sign of the wave vector  $k$ .

In the three tests described above, although some oscillations occur when crossing the interfaces  $x = -1$  and  $x = 1$ , the quantitative comparison gives also good results. In particular, we represented in Figure 4 the variation with respect to  $\operatorname{Im} \theta_0$  of the maximum in time of the  $L^2$  relative difference:

$$D_{\theta_0} = \max_{1 \leq n \leq N} 100 \frac{\|u_{\theta_0}^n - u^n\|}{\|u_I\|}, \quad (2.21)$$

where  $N = 400$  is the number of time iterations. It shows that, for every case, the difference tends to 0 when  $\operatorname{Im} \theta_0$  tends to 0. Moreover, the graphic of  $D_{\theta_0}$  is a line which validates the result (2.14). We note also that the difference in the case of a barrier potential is smaller than in the case  $V = 0$ . This may be due to the fact that the error coming from the interface conditions is compensated by the exponential decay imposed by the barrier. Then, in the case of a barrier potential, we note that the difference is more important when the initial condition is supported in  $(-1, 1)$ . It can be explained by the fact that the solution crosses the two interfaces, at  $x = -1$  and  $x = 1$ , whereas, when the solution comes from the left, only the interaction with the first interface  $x = -1$  is relevant, which is also a consequence of the exponential decay in the barrier.

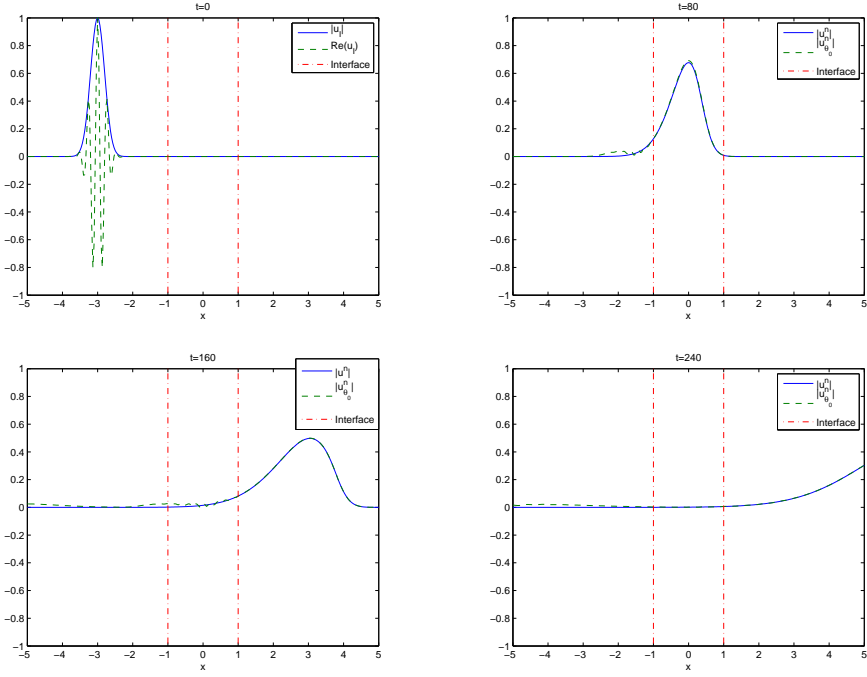


Figure 1: Case  $V = 0$ : modulus of the functions  $u^n_{\theta_0}$  and  $u^n$  at different time  $t$  with  $x_0 = -3$  and  $\theta_0 = 0.09i$

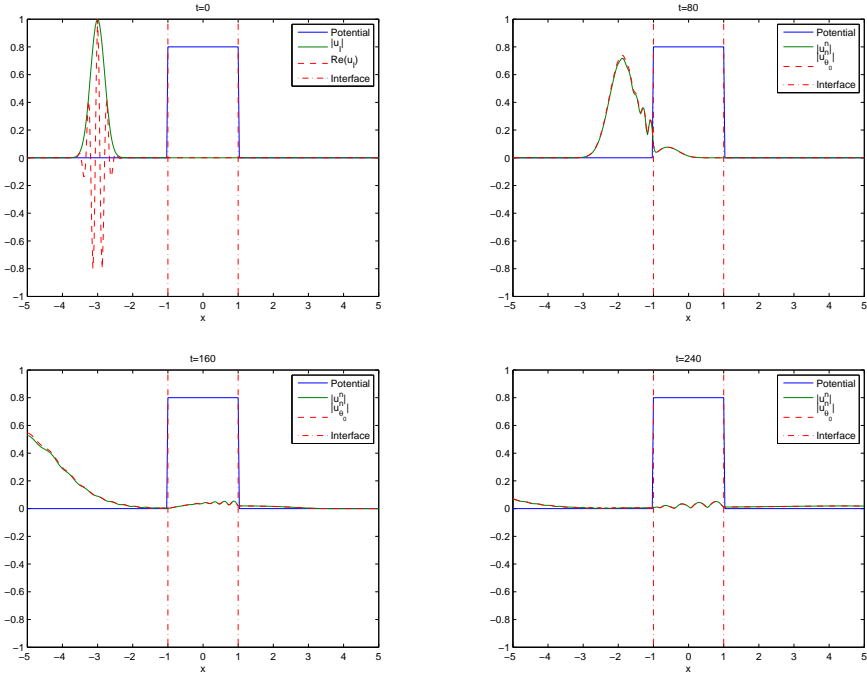


Figure 2: Case of a barrier potential: modulus of the functions  $u^n_{\theta_0}$  and  $u^n$  at different time  $t$  with  $x_0 = -3$  and  $\theta_0 = 0.09i$

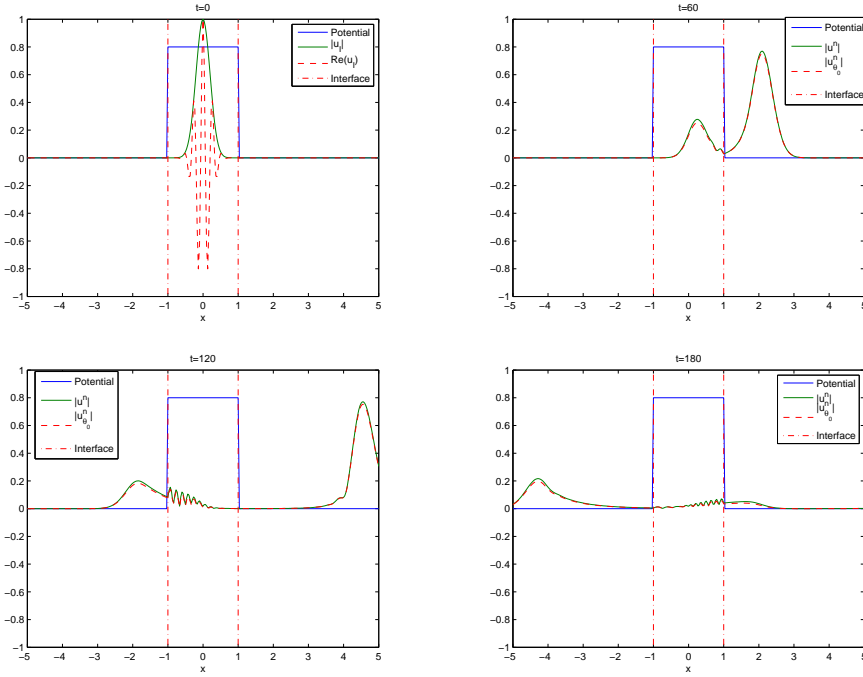


Figure 3: Case of a barrier potential: modulus of the functions  $u_{\theta_0}^n$  and  $u^n$  at different time  $t$  with  $x_0 = 0$  and  $\theta_0 = 0.09i$

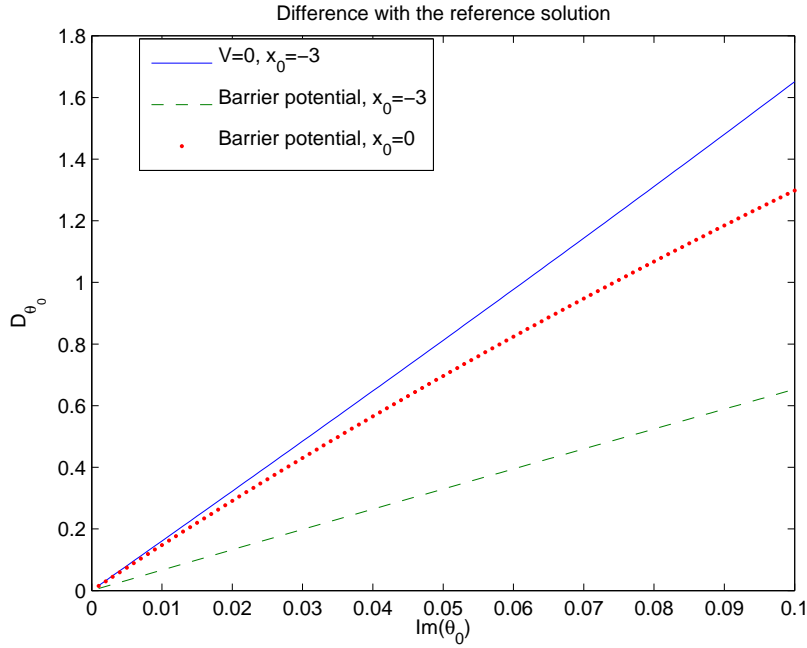


Figure 4: Variation with respect to  $\text{Im } \theta_0$  of the difference  $D_{\theta_0}$ , defined in (2.21), in the case  $V = 0$  with  $x_0 = -3$ , and in the case of a barrier potential with  $x_0 = -3$  and  $x_0 = 0$

### 3 Exterior complex scaling and local perturbations

Spectral deformations of Schrödinger operators arising from complex dilations form a standard tool to study resonances. This technique – originally developed by J.M. Combes and coauthors in [3][10] for the homogeneous scaling in  $L^2(\mathbb{R}^n)$ :  $U_\theta\psi(x) = e^{\frac{\theta}{2}}\psi(e^\theta x)$  – allows to relate the resonances of the Hamiltonian  $H = -\Delta + \mathcal{V}$  with the spectral points of a non self-adjoint operator  $H(\theta) = U_\theta H U_\theta^{-1}$  with  $\theta \in \mathbb{C}$ . If the potential  $\mathcal{V}$  is *dilation analytic* in the strip  $\{\theta \in \mathbb{C} \mid |\operatorname{Im} \theta| < \alpha\}$ , the poles of the meromorphic continuation of the resolvent  $(H - z)^{-1}$  in the second Riemann sheet are identified with the eigenvalues of  $H(\theta)$  placed in the cone spanned by the positive real axis and the rotated half axis  $e^{-2i\operatorname{Im} \theta}\mathbb{R}_+$ . We refer the reader to [23] for a summary and we recall that many variations on this approach have been developed since, see [31][30][40] and [29] for a short comparison of these methods. In particular for potentials which can be complex deformed only outside a compact region, the exterior complex scaling technique appeared first in [54] in the singular version that we reconsider here. Meanwhile regular versions have been used in [31] and extended with the so called “black box” formalism in [56].

In this section, we consider a particular class of exterior scaling maps,  $U_\theta$ , acting outside a compact set in 1D and introducing sharp singularities in the domain of the corresponding deformed Hamiltonians. Let us introduce the one-parameter family of exterior dilations

$$x \longrightarrow \begin{cases} e^{-\theta}(x - b) + b, & x > b \\ x, & x \in (a, b) \\ e^{-\theta}(x - a) + a, & x < a. \end{cases} \quad (3.1)$$

For real values of the parameter  $\theta$ , the related unitary transformation in  $L^2(\mathbb{R})$  is

$$U_\theta\psi(x) = \begin{cases} e^{\frac{\theta}{2}}\psi(e^\theta(x - b) + b), & x > b \\ \psi(x), & x \in (a, b) \\ e^{\frac{\theta}{2}}\psi(e^\theta(x - a) + a), & x < a. \end{cases} \quad (3.2)$$

Local perturbations of  $H_{\theta_0,0}^h(0)$  are defined by

$$H_{\theta_0,\mathcal{V}}^h(0) = H_{\theta_0,0}^h(0) + \mathcal{V}, \quad (3.3)$$

with  $\operatorname{supp} \mathcal{V} \subset [a, b]$ . In what follows we will assume

$$\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2, \quad \mathcal{V}_1 \in L^\infty((a, b)), \quad \mathcal{V}_2 \in \mathcal{M}_b(U) \quad \text{with } U \subset\subset (a, b). \quad (3.4)$$

Under these assumptions,

$$D(H_{\theta_0,\mathcal{V}}^h(0)) = \{u \in H^2(\mathbb{R} \setminus \{a, b, U\}) \mid (1 - \chi)u \in D(H_{\theta_0,0}^h(0)), -h^2 u'' + \mathcal{V}_2 u \in L^2(U)\},$$

where  $\chi \in C_0^\infty((a, b))$  and  $\chi(x) = 1$  for  $x \in U$ .

In particular, since  $\mathcal{V}_2$  is a bounded measure, the domain  $D(H_{\theta_0,\mathcal{V}}^h(0))$  is contained in  $H^1(\mathbb{R} \setminus \{a, b\})$ . The conjugated operator

$$H_{\theta_0,\mathcal{V}}^h(\theta) = U_\theta H_{\theta_0,\mathcal{V}}^h(0) U_\theta^{-1} \quad (3.5)$$

is defined on  $D(H_{\theta_0,\mathcal{V}}^h(\theta)) = \left\{u \in L^2(\mathbb{R}) \mid U_\theta^{-1}u \in D(H_{\theta_0,\mathcal{V}}^h(0))\right\}$ . The constraint  $U_\theta^{-1}u \in D(H_{\theta_0,\mathcal{V}}^h(0))$  compels the boundary conditions

$$\begin{cases} e^{-\frac{1}{2}(\theta_0+\theta)}u(b^+) = u(b^-); & e^{-\frac{3}{2}(\theta_0+\theta)}u'(b^+) = u'(b^-) \\ e^{-\frac{1}{2}(\theta_0+\theta)}u(a^-) = u(a^+); & e^{-\frac{3}{2}(\theta_0+\theta)}u'(a^-) = u'(a^+), \end{cases} \quad (3.6)$$

to hold for any  $u \in D(H_{\theta_0,\mathcal{V}}^h(\theta))$ . Thus one has

$$D(H_{\theta_0,\mathcal{V}}^h(\theta)) = \{u \in H^2(\mathbb{R} \setminus \{a, b, U\}) \cap H^1(\mathbb{R} \setminus \{a, b\}) \mid (3.6), -h^2 u'' + \mathcal{V}_2 u \in L^2(U)\}. \quad (3.7)$$

The action of  $H_{\theta_0, \mathcal{V}}^h(\theta)$  is

$$H_{\theta_0, \mathcal{V}}^h(\theta)u = [-h^2\eta(x)\partial_x^2 + \mathcal{V}] u, \quad \eta(x) = e^{-2\theta \mathbf{1}_{\mathbb{R} \setminus (a, b)}(x)}. \quad (3.8)$$

It is worthwhile to notice that this definition can be extended to complex values of  $\theta$ . For  $\theta \in \mathbb{C}$ , the Hamiltonian  $H_{\theta_0, \mathcal{V}}^h(\theta)$  identifies with a restriction of the operator  $Q(\theta)$

$$\begin{cases} D(Q(\theta)) = \{u \in H^2(\mathbb{R} \setminus \{a, b, U\}) \cap H^1(\mathbb{R} \setminus \{a, b\}) \mid -h^2u'' + \mathcal{V}_2u \in L^2(U)\}, \\ Q(\theta)u = [-h^2\eta(x)\partial_x^2 + \mathcal{V}] u. \end{cases} \quad (3.9)$$

For particular choices of  $\theta_0$  and  $\theta$ , the quantum evolution generated by the deformed model  $H_{\theta_0, \mathcal{V}}^h(\theta)$  is described by contraction maps. To fix this point, let us consider the terms  $\operatorname{Re} \langle u, iH_{\theta_0, \mathcal{V}}^h(\theta)u \rangle_{L^2(\mathbb{R})}$ ; for  $u \in D(H_{\theta_0, \mathcal{V}}^h(\theta))$ , an explicit calculation gives

$$\begin{aligned} \operatorname{Re} \langle u, iH_{\theta_0, \mathcal{V}}^h(\theta)u \rangle_{L^2(\mathbb{R})} &= \operatorname{Re} \left\{ -ih^2 (\bar{u}(a^-)u'(a^-) - \bar{u}(b^+)u'(b^+)) \left( e^{-2\theta} - e^{-\frac{1}{2}(\bar{\theta} + \bar{\theta}_0)} e^{-\frac{3}{2}(\theta + \theta_0)} \right) \right\} \\ &\quad + h^2 e^{-2\operatorname{Re} \theta} \sin(2\operatorname{Im} \theta) \int_{\mathbb{R} \setminus (a, b)} |u'|^2 dx. \end{aligned} \quad (3.10)$$

For  $\theta = \theta_0 = i\tau$ , with  $\tau \in (0, \frac{\pi}{2})$ , the boundary terms disappear, and the r.h.s. of (3.10) is positive

$$\operatorname{Re} \langle u, iH_{i\tau, \mathcal{V}}^h(i\tau)u \rangle_{L^2(\mathbb{R})} = h^2 \sin(2\tau) \int_{\mathbb{R} \setminus (a, b)} |u'|^2 dx \geq 0. \quad (3.11)$$

**Lemma 3.1.** *For  $\tau \in (0, \frac{\pi}{2})$ , the operator  $iH_{i\tau, \mathcal{V}}^h(i\tau)$  is the generator of a contraction semigroup.*

**Proof:** As a consequence of (3.11),  $iH_{i\tau, \mathcal{V}}^h(i\tau)$  is accretive. Moreover, the propriety  $\sigma_{ess}(H_{i\tau, \mathcal{V}}^h(i\tau)) = e^{-2i\tau}\mathbb{R}_+$  in Corollary 3.4 below, implies  $i\lambda_0 \in \rho(H_{i\tau, \mathcal{V}}^h(i\tau))$  for some  $\lambda_0 > 0$  and  $(iH_{i\tau, \mathcal{V}}^h(i\tau) + \lambda_0)$  is surjective. Then, a standard characterization of semigroup generators ([51], Theorem X.48) leads to the result.  $\square$

### 3.1 Krein formula and analyticity of the resolvent

In order to get an expression of the adjoint operator of  $H_{\theta_0, \mathcal{V}}^h(\theta)$ , we introduce the following operator with two-parameters boundary conditions

$$D(\mathcal{Q}_{\theta_1, \theta_2}(\theta)) = \left\{ u \in D(Q(\theta)) \mid \begin{cases} e^{-\frac{1}{2}(\theta_1 + \theta)}u(b^+) = u(b^-); & e^{-\frac{1}{2}(\theta_2 + 3\theta)}u'(b^+) = u'(b^-) \\ e^{-\frac{1}{2}(\theta_1 + \theta)}u(a^-) = u(a^+); & e^{-\frac{1}{2}(\theta_2 + 3\theta)}u'(a^-) = u'(a^+) \end{cases} \right\}, \quad (3.12)$$

$$\mathcal{Q}_{\theta_1, \theta_2}(\theta)u = [-h^2\eta(x)\partial_x^2 + \mathcal{V}] u, \quad \eta(x) = e^{-2\theta \mathbf{1}_{\mathbb{R} \setminus (a, b)}(x)}, \quad (3.13)$$

where  $Q(\theta)$  is defined in (3.9). Indeed, by direct computation

i)  $\mathcal{Q}_{\theta_1, \theta_2}(\theta)$  identifies with the original model  $H_{\theta_0, \mathcal{V}}^h(\theta)$  for the choice of parameters:  $\theta_1 = \theta_0$  and  $\theta_2 = 3\theta_0$

$$H_{\theta_0, \mathcal{V}}^h(\theta) = \mathcal{Q}_{\theta_0, 3\theta_0}(\theta), \quad (3.14)$$

ii) the adjoint operator  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta))^*$  is given by

$$(\mathcal{Q}_{\theta_1, \theta_2}(\theta))^* = \mathcal{Q}_{-\bar{\theta}_2, -\bar{\theta}_1}(\bar{\theta}). \quad (3.15)$$

Like  $H_{\theta_0, \mathcal{V}}^h(\theta)$ , the Hamiltonian  $\mathcal{Q}_{\theta_1, \theta_2}(\theta)$  is a restriction of the operator  $Q(\theta)$ . In this context, we fix a boundary value triple  $\{\Gamma_{j=1,2}^\theta, \mathbb{C}^4\}$  with  $\Gamma_j^\theta : D(Q(\theta)) \rightarrow \mathbb{C}^4$

$$\Gamma_1^\theta \psi = h^2 \begin{pmatrix} -e^{-\frac{3}{2}\theta} \psi'(b^+) \\ -\psi(b^-) \\ \psi(a^+) \\ e^{-\frac{3}{2}\theta} \psi'(a^-) \end{pmatrix}; \quad \Gamma_2^\theta \psi = \begin{pmatrix} e^{-\frac{\theta}{2}} \psi(b^+) \\ \psi'(b^-) \\ \psi'(a^+) \\ e^{-\frac{\theta}{2}} \psi(a^-) \end{pmatrix}, \quad (3.16)$$

and  $(\Gamma_1^\theta, \Gamma_2^\theta) : D(Q(\theta)^*) \rightarrow \mathbb{C}^4 \times \mathbb{C}^4$  surjective. For all  $\psi, \varphi \in D(Q(\theta))$ , these maps satisfy the relation

$$\langle \psi, Q(\theta)\varphi \rangle_{L^2(\mathbb{R})} - \langle Q(\bar{\theta})\psi, \varphi \rangle_{L^2(\mathbb{R})} = \langle \Gamma_1^{\bar{\theta}}\psi, \Gamma_2^\theta\varphi \rangle_{\mathbb{C}^4} - \langle \Gamma_2^{\bar{\theta}}\psi, \Gamma_1^\theta\varphi \rangle_{\mathbb{C}^4} \quad (3.17)$$

(for the definition of boundary triples and the construction of point interaction potentials in the self adjoint case see [47] and [4]). Let  $\Lambda, B \in \mathbb{C}^{4,4}$  be defined as

$$\Lambda(\theta_1, \theta_2) = \frac{1}{h^2} \begin{pmatrix} a(\theta_1, \theta_2) & \\ & -a(-\theta_2, -\theta_1) \end{pmatrix}, \quad B = \begin{pmatrix} b & \\ & b \end{pmatrix}, \quad (3.18)$$

$$a(\theta_1, \theta_2) = \begin{pmatrix} -e^{-\frac{\theta_2}{2}} & 0 \\ 0 & -e^{\frac{\theta_1}{2}} \end{pmatrix}, \quad b = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (3.19)$$

the boundary conditions in (3.12) are equivalent to

$$\Lambda \Gamma_1^\theta \psi = B \Gamma_2^\theta \psi. \quad (3.20)$$

Let  $H_{ND, \mathcal{V}}^h(\theta)$  denote the restriction of  $Q(\theta)$  corresponding to the boundary conditions:  $\Gamma_1^\theta \psi = 0$ ; this operator is explicitly given by

$$H_{ND, \mathcal{V}}^h(\theta) = -h^2 e^{-2\theta} \Delta_{(-\infty, a)}^N \oplus \left[ -h^2 \Delta_{(a, b)}^D + \mathcal{V} \right] \oplus -h^2 e^{-2\theta} \Delta_{(b, +\infty)}^N. \quad (3.21)$$

Its spectrum is characterized as follows

$$\sigma(H_{ND, \mathcal{V}}^h(\theta)) = e^{-2\theta} \mathbb{R}_+ \cup \sigma(-h^2 \Delta_{(a, b)}^D + \mathcal{V}). \quad (3.22)$$

It is possible to write  $(Q_{\theta_1, \theta_2}(\theta) - z)^{-1}$  as the sum of  $(H_{ND, \mathcal{V}}^h(\theta) - z)^{-1}$  plus finite rank terms. Such a representation will be further used to develop the spectral analysis of  $H_{\theta_0, \mathcal{V}}^h(\theta)$  where our Krein-like formula will allow explicit resolvent estimates near the resonances. The space  $\mathcal{N}_{z, \theta} = \text{Ker}(Q(\theta) - z)$  is generated by the linear closure of the system  $\{u_{i, z}\}_{i=1}^4$  where  $u_{i, z}$  are the independent solutions to  $(Q(\theta) - z)u = 0$ . The exterior solutions to this problem,  $u_{i, z}$ ,  $i = 1, 4$ , are explicitly given by

$$u_{1, z}(x) = 1_{(b, +\infty)} e^{i \frac{\sqrt{ze^{2\theta}}}{h} (x-b)}, \quad u_{4, z}(x) = 1_{(-\infty, a)} e^{-i \frac{\sqrt{ze^{2\theta}}}{h} (x-a)}, \quad (3.23)$$

where the square root branch cut is fixed with  $\text{Im} \sqrt{\cdot} > 0$ . This assumption implies  $\text{Im} \sqrt{ze^{2\theta}} > 0$  for all  $z \in \mathbb{C} \setminus e^{-2i \text{Im} \theta} \mathbb{R}_+$ . The interior solutions,  $u_{i, z}$ ,  $i = 2, 3$ , can be defined through the following boundary value problems

$$\begin{cases} [-h^2 \partial_x^2 + \mathcal{V} - z] u_{2, z} = 0, & \text{in } (a, b), \\ u_{2, z}(a) = 0, \quad u_{2, z}(b) = 1, \end{cases} \quad \begin{cases} [-h^2 \partial_x^2 + \mathcal{V} - z] u_{3, z} = 0, & \text{in } (a, b), \\ u_{3, z}(a) = 1, \quad u_{3, z}(b) = 0, \end{cases} \quad (3.24)$$

with  $z \in \mathbb{C} \setminus \sigma_p(H_{ND, \mathcal{V}}^h(\theta))$ . Owing to the property of the interior Dirichlet realization in  $(a, b)$ , the solutions  $u_{i, z}|_{(a, b)}$  are unique and locally  $H^2$  near the boundary. We consider the maps:  $\gamma(\cdot, z, \theta) = \left( \Gamma_1^\theta|_{\mathcal{N}_{z, \theta}} \right)^{-1}$ , with  $\Gamma_1^\theta|_{\mathcal{N}_{z, \theta}}$  denoting the restriction of  $\Gamma_1^\theta$  onto  $\mathcal{N}_{z, \theta}$ , and  $q(z, \theta, \mathcal{V}) = \Gamma_2^\theta \gamma(\cdot, z, \theta)$ . These form holomorphic families of linear operators for  $z$  in a cut plane  $\mathbb{C} \setminus e^{-2i \text{Im} \theta} \mathbb{R}_+$ . Their matrix form w.r.t. the standard basis  $\{\varepsilon_j\}_{j=1}^4$  of  $\mathbb{C}^4$  and the system  $\{u_{i, z}\}_{i=1}^4$  is:  $\gamma_{ij}(z, \theta) = c_i(z, \theta) \delta_{ij}$  with

$$c_1(z, \theta) = \frac{ie^{\frac{3\theta}{2}}}{h\sqrt{ze^{2\theta}}}, \quad c_2 = -\frac{1}{h^2}, \quad c_3 = \frac{1}{h^2}, \quad c_4(z, \theta) = \frac{ie^{\frac{3\theta}{2}}}{h\sqrt{ze^{2\theta}}}, \quad (3.25)$$

and

$$q(z, \theta, \mathcal{V}) = \frac{1}{h^2} \begin{pmatrix} \frac{ih e^\theta}{\sqrt{ze^{2\theta}}} & & & \\ & -u'_{2, z}(b) & u'_{3, z}(b) & \\ & -u'_{2, z}(a) & u'_{3, z}(a) & \\ & & & \frac{ih e^\theta}{\sqrt{ze^{2\theta}}} \end{pmatrix}. \quad (3.26)$$

**Lemma 3.2.** Let  $\varphi \in L^2(\mathbb{R})$  and  $j = 1, \dots, 4$ ; the relation

$$\left[ \Gamma_2^\theta (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi \right]_j = \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})} \quad (3.27)$$

holds with  $\theta \in \mathbb{C}$  and  $z \in \rho(H_{ND,\mathcal{V}}^h(\theta))$ .

**Proof:** Let:  $f = (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi$ . This function is in  $D(H_{ND,\mathcal{V}}^h(\theta))$  so that:  $Q(\theta)f = H_{ND,\mathcal{V}}^h(\theta)f$  and  $\Gamma_1^\theta f = 0$ . The l.h.s of (3.27) writes as

$$\left[ \Gamma_2^\theta (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi \right]_j = \langle \underline{e}_j, \Gamma_2^\theta f \rangle_{\mathbb{C}^4}.$$

Since  $\underline{e}_j = \Gamma_1^{\bar{\theta}} \gamma(\underline{e}_j, \bar{z}, \bar{\theta})$ , we have

$$\begin{aligned} \left[ \Gamma_2^\theta (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi \right]_j &= \left\langle \Gamma_1^{\bar{\theta}} \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \Gamma_2^\theta f \right\rangle_{\mathbb{C}^4} - \left\langle \Gamma_2^{\bar{\theta}} \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \Gamma_1^\theta f \right\rangle_{\mathbb{C}^4} \\ &= \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), Q(\theta)f \rangle_{L^2(\mathbb{R})} - \langle Q(\bar{\theta})\gamma(\underline{e}_j, \bar{z}, \bar{\theta}), f \rangle_{L^2(\mathbb{R})}. \end{aligned}$$

By definition,  $\gamma(\underline{e}_j, \bar{z}, \bar{\theta}) \in \mathcal{N}_{\bar{z}, \bar{\theta}}$  and the r.h.s. writes as

$$\begin{aligned} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), Q(\theta)f \rangle_{L^2(\mathbb{R})} - \langle Q(\bar{\theta})\gamma(\underline{e}_j, \bar{z}, \bar{\theta}), f \rangle_{L^2(\mathbb{R})} &= \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), (H_{ND,\mathcal{V}}^h(\theta) - z)f \rangle_{L^2(\mathbb{R})} \\ &= \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})}. \end{aligned}$$

□

**Proposition 3.3.** The resolvent  $(Q_{\theta_1, \theta_2}(\theta) - z)^{-1}$  allows the representation

$$\begin{aligned} (Q_{\theta_1, \theta_2}(\theta) - z)^{-1} &= (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \\ &\quad - \sum_{i,j=1}^4 \left[ (Bq(z, \theta, \mathcal{V}) - \Lambda)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta), \end{aligned} \quad (3.28)$$

and one has:  $\sigma_{ess}(Q_{\theta_1, \theta_2}(\theta)) = \sigma_{ess}(H_{ND,\mathcal{V}}^h(\theta)) = e^{-2\theta} \mathbb{R}_+$ .

**Proof:** Let us consider the r.h.s. of this formula: the operator  $(H_{ND,\mathcal{V}}^h(\theta) - z)^{-1}$  is well defined for  $z \in \mathbb{C} \setminus \sigma(H_{ND,\mathcal{V}}^h(\theta))$ . The vectors  $\gamma(\underline{e}_i, z, \theta)$ ,  $i = 1, \dots, 4$ , are given by (3.23), (3.24), (3.25), while the boundary values of  $u'_{i,z}$  – appearing in the definition of the matrix (3.26) – are well defined whenever  $z \in \mathbb{C} \setminus \sigma_p(H_{ND,\mathcal{V}}^h(\theta))$ . Therefore, the r.h.s. of (3.28) makes sense for  $z \in \mathbb{C} \setminus \{\sigma(H_{ND,\mathcal{V}}^h(\theta)) \cup \mathcal{T}_0\}$  where  $\mathcal{T}_0$  is the (at most) discrete set, described by the transcendental equation

$$\det(Bq(z, \theta, \mathcal{V}) - \Lambda(\theta_1, \theta_2)) = 0. \quad (3.29)$$

It is worthwhile to notice that  $\mathbb{C} \setminus \{\sigma(H_{ND,\mathcal{V}}^h(\theta)) \cup \mathcal{T}_0\}$  is not empty. Let us introduce the map  $R_z(\varphi)$  defined for  $\varphi \in L^2(\mathbb{R})$  by

$$\begin{aligned} R_z(\varphi) &= \phi - \psi, \\ \phi &= (H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi, \\ \psi &= \sum_{i,j=1}^4 \left[ (Bq(z, \theta, \mathcal{V}) - \Lambda)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta), \end{aligned}$$

with  $q(z, \theta, \mathcal{V})$  given in (3.26) and  $z \in \rho(H_{ND,\mathcal{V}}^h(\theta)) \setminus \mathcal{T}_0$ . In what follows we show that:

$R_z(\varphi) = (Q_{\theta_1, \theta_2}(\theta) - z)^{-1} \varphi$ . Since  $H_{ND,\mathcal{V}}^h(\theta) \subset Q(\theta)$  and  $\gamma(\underline{e}_i, z, \theta) \in \text{Ker}(Q(\theta) - z)$ , one has:

$$(H_{ND,\mathcal{V}}^h(\theta) - z)^{-1} \varphi, \gamma(\underline{e}_i, z, \theta) \in D(Q(\theta)).$$

This implies  $R_z(\varphi) \in D(Q(\theta))$ . To simplify the presentation, we will temporarily use the notation  $q = q(z, \theta, \mathcal{V})$ . Being  $\phi \in D(H_{ND, \mathcal{V}}^h(\theta))$ , we have:  $\Gamma_1^\theta \phi = 0$  and the following relation holds

$$(Bq - \Lambda) \Gamma_1^\theta (\phi - \psi) = - (B\Gamma_2^\theta \gamma(\cdot, z, \theta) - \Lambda) \Gamma_1^\theta \psi = (-B\Gamma_2^\theta + \Lambda \Gamma_1^\theta) \psi, \quad (3.30)$$

where  $\psi \in \mathcal{N}_{z, \theta}$  and

$$\gamma(\cdot, z, \theta) \Gamma_1^\theta|_{\mathcal{N}_{z, \theta}} = 1$$

have been used. At the same time, the  $n$ -th component of the vector at the l.h.s. can be expressed as

$$\begin{aligned} [(Bq - \Lambda) \Gamma_1^\theta (\phi - \psi)]_n &= [- (Bq - \Lambda) \Gamma_1^\theta \psi]_n \\ &= - \sum_{i,j=1}^4 [(Bq - \Lambda) \Gamma_1^\theta \gamma(\underline{e}_i, z, \theta)]_n \left[ (Bq - \Lambda)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})}. \end{aligned}$$

Recalling that  $\Gamma_1^\theta \gamma(\underline{e}_i, z, \theta) = e_i$ , we get

$$\begin{aligned} [(Bq - \Lambda) \Gamma_1^\theta (\phi - \psi)]_n &= \\ &= - \sum_{i,j=1}^4 (Bq - \Lambda)_{ni} \left[ (Bq - \Lambda)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})} = - \sum_{j=1}^4 B_{nj} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \varphi \rangle_{L^2(\mathbb{R})}. \end{aligned}$$

Taking into account the result of the Lemma 3.2, this relation writes as

$$(Bq - \Lambda) \Gamma_1^\theta (\phi - \psi) = -B\Gamma_2^\theta \phi. \quad (3.31)$$

Combining (3.30) and (3.31), one has:  $-\Lambda \Gamma_1^\theta \psi = B\Gamma_2^\theta (\phi - \psi)$ , and, adding the null term  $\Lambda \Gamma_1^\theta \phi$  at the l.h.s.,

$$\Lambda \Gamma_1^\theta R_z(\varphi) = B\Gamma_2^\theta R_z(\varphi),$$

which, according to (3.20), is the boundary condition characterizing  $\mathcal{Q}_{\theta_1, \theta_2}(\theta)$  as a restriction of  $Q(\theta)$ . Then we have:  $R_z(\varphi) \in D(\mathcal{Q}_{\theta_1, \theta_2}(\theta))$ . Furthermore,

$$(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z) R_z(\varphi) = (Q(\theta) - z) R_z(\varphi) = \varphi - (Q(\theta) - z) \psi = \varphi, \quad (3.32)$$

where  $(Q(\theta) - z) \gamma(\underline{e}_i, z, \theta) = 0$  has been used. This leads to the surjectivity of the operator  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)$  for any  $z \in \mathbb{C} \setminus \{\sigma(H_{ND, \mathcal{V}}^h(\theta)) \cup \mathcal{T}_0\}$ . The injectivity is obtained using the adjoint of  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)$ . Indeed, the equality (3.15) implies

$$(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)^* = (\mathcal{Q}_{-\bar{\theta}_2, -\bar{\theta}_1}(\bar{\theta}) - \bar{z}),$$

which, from the result above, appears to be surjective for all  $z$  such that  $\bar{z} \in \mathbb{C} \setminus \{\sigma(H_{ND, \mathcal{V}}^h(\bar{\theta})) \cup \tilde{\mathcal{T}}_0\}$ , where  $\tilde{\mathcal{T}}_0$  is the discrete set of the solutions to (3.29) when replacing:  $\theta = \bar{\theta}$ ,  $\theta_1 = -\bar{\theta}_2$  and  $\theta_2 = -\bar{\theta}_1$ . As a consequence of (3.22), we have

$$\bar{z} \in \sigma(H_{ND, \mathcal{V}}^h(\bar{\theta})) \Leftrightarrow z \in \sigma(H_{ND, \mathcal{V}}^h(\theta)).$$

It follows that for any  $z \in \mathbb{C} \setminus \{\sigma(H_{ND, \mathcal{V}}^h(\theta)) \cup \mathcal{T}\}$ , where  $\mathcal{T} = \mathcal{T}_0 \cup \{z \text{ s.t. } \bar{z} \in \tilde{\mathcal{T}}_0\}$ , the operator  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)$  is surjective and

$$\text{Ker}(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z) = [\text{Ran}(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)^*]^\perp = \{0\}.$$

We get that  $\forall z \in \mathbb{C} \setminus \{\sigma(H_{ND, \mathcal{V}}^h(\theta)) \cup \mathcal{T}\}$ ,  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)$  is invertible and  $(\mathcal{Q}_{\theta_1, \theta_2}(\theta) - z)^{-1} = R_z$ . Moreover, for such a complex  $z$ , the difference  $R_z - (H_{ND, \mathcal{V}}^h(\theta) - z)^{-1}$  is compact. Then, we conclude that

$$\sigma_{ess}(\mathcal{Q}_{\theta_1, \theta_2}(\theta)) = \sigma_{ess}(H_{ND, \mathcal{V}}^h(\theta)) = e^{-2\theta} \mathbb{R}_+$$



(for this point, we refer to [52], Sec. XIII.4, Lemma 3 and the strong spectral mapping theorem), and the equality (3.28) holds as an identity of meromorphic functions on  $\mathbb{C} \setminus e^{-2\theta}\mathbb{R}_+$ .  $\square$

As a direct consequence of the previous proposition and the identification (3.14), the representation of the resolvent  $(H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1}$  is obtained by replacing the matrix  $\Lambda$  in (3.28) by the matrix  $A = \Lambda(\theta_0, 3\theta_0)$  where the matrix  $\Lambda(\theta_1, \theta_2)$  is given in (3.18). It follows that for the matrices

$$A = \frac{1}{h^2} \begin{pmatrix} -e^{-\frac{3}{2}\theta_0} & & & \\ & -e^{\frac{\theta_0}{2}} & & \\ & & e^{\frac{\theta_0}{2}} & \\ & & & e^{-\frac{3}{2}\theta_0} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & & \\ 1 & 0 & & \\ & & 0 & 1 \\ & & 1 & 0 \end{pmatrix}, \quad (3.33)$$

the result below holds.

**Corollary 3.4.** *Let  $\mathcal{V}$  and  $A, B$  be defined as in (3.4) and (3.33). The resolvent  $(H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1}$  allows the representation*

$$(H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1} = (H_{ND, \mathcal{V}}^h(\theta) - z)^{-1} - \sum_{i,j=1}^4 \left[ (Bq(z, \theta, \mathcal{V}) - A)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta), \quad (3.34)$$

and one has:  $\sigma_{ess}(H_{\theta_0, \mathcal{V}}^h(\theta)) = \sigma_{ess}(H_{ND, \mathcal{V}}^h(\theta)) = e^{-2\theta}\mathbb{R}_+$ .

The analyticity of the resolvent  $(H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1}$  w.r.t.  $\theta$  is an important point in the theory of resonances. The former is obtained in the next proposition as a consequence of the formula (3.34), the latter is developed in the next section.

**Proposition 3.5.** *Consider  $\theta_0 \in \mathbb{C}$ ,  $\mathcal{V}$  fulfilling the conditions (3.4), and let  $S_\alpha = \{\theta \in \mathbb{C} \mid |\operatorname{Im} \theta| \leq \alpha\}$  for positive  $\alpha < \frac{\pi}{4}$ . Then, there exists an open subset  $\mathcal{O} \subset \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\}$  such that  $\forall \theta \in S_\alpha$ ,  $\mathcal{O} \subset \rho(H_{\theta_0, \mathcal{V}}^h(\theta))$ . Moreover,  $\forall z \in \mathcal{O}$ , the map:  $\theta \mapsto (H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1}$  is a bounded operator-valued analytic map on the strip  $S_\alpha$ .*

Before starting the proof, we note that this result implies that the  $\theta$  dependent family of operators  $H_{\theta_0, \mathcal{V}}^h(\theta)$  is analytic in the sense of Kato in the strip  $S_\alpha$  (definition in [52]).

**Proof:** The equality (3.34) holding as an identity of meromorphic functions on  $\mathbb{C} \setminus e^{-2\theta}\mathbb{R}_+$ , the poles on the l.h.s. identifies with those on the r.h.s.. For  $\theta \in S_\alpha$ , the characterization (3.22) implies that the map  $z \mapsto (H_{ND, \mathcal{V}}^h(\theta) - z)^{-1}$  is analytic when  $\operatorname{Re} z < 0$ . It results

$$\sigma(H_{\theta_0, \mathcal{V}}^h(\theta)) \cap \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\} = \mathcal{T}_0 \cap \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\},$$

where

$$\mathcal{T}_0 = \{z \in \mathbb{C} \mid \det(Bq(z, \theta, \mathcal{V}) - A) = 0\}.$$

Noting that for  $\operatorname{Re} z < 0$  and  $\theta \in S_\alpha$  we have  $\sqrt{ze^{2\theta}} = \sqrt{z}e^\theta$ , and therefore  $q(z, \theta, \mathcal{V}) = q(z, 0, \mathcal{V})$ , we get:  $\forall \theta \in S_\alpha$

$$\sigma(H_{\theta_0, \mathcal{V}}^h(\theta)) \cap \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\} = \{z \in \mathbb{C} \mid \operatorname{Re} z < 0 \text{ and } \det(Bq(z, 0, \mathcal{V}) - A) = 0\},$$

which is a discrete set independent of  $\theta$ . This implies that there exists an open subset  $\mathcal{O} \subset \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\}$  such that  $\forall \theta \in S_\alpha$ ,  $\mathcal{O} \subset \rho(H_{\theta_0, \mathcal{V}}^h(\theta))$ .

In what follows, we fix  $z \in \mathcal{O}$ . The equation (3.34) gives, for any  $\theta \in S_\alpha$

$$(H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1} = (H_{ND, \mathcal{V}}^h(\theta) - z)^{-1} - \sum_{i,j=1}^4 \left[ (Bq(z, 0, \mathcal{V}) - A)^{-1} B \right]_{ij} \langle \gamma(\underline{e}_j, \bar{z}, \bar{\theta}), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta), \quad (3.35)$$

where we used  $q(z, \theta, \mathcal{V}) = q(z, 0, \mathcal{V})$ , and we want to study the analyticity of the r.h.s. with respect to  $\theta$ .

Let us start with the operator  $H_{ND, \mathcal{V}}^h(\theta)$ :  $\forall \theta \in S_\alpha$ , it is a closed operator with non empty resolvent set. Moreover,  $D(H_{ND, \mathcal{V}}^h(\theta))$  does not depend on  $\theta$  and  $\forall \psi \in D(H_{ND, \mathcal{V}}^h(\theta)), \forall f \in L^2(\mathbb{R})$  the map

$$\theta \mapsto \langle f, H_{ND, \mathcal{V}}^h(\theta) \psi \rangle_{L^2(\mathbb{R})}$$

is analytic on  $S_\alpha$ . This means that  $H_{ND, \mathcal{V}}^h(\theta)$  is analytic of type (A) following the definition in [52]. In addition, since  $\operatorname{Re} z < 0$  when  $z \in \mathcal{O}$ , (3.22) implies  $z \in \rho(H_{ND, \mathcal{V}}^h(\theta))$  for all  $\theta \in S_\alpha$ . Then, it results from the analyticity of type (A) propriety that the map  $\theta \mapsto (H_{ND, \mathcal{V}}^h(\theta) - z)^{-1}$  is analytic on  $S_\alpha$ .

Concerning the finite rank part in (3.35), for any  $z$  with  $\operatorname{Re} z < 0$ , the functions  $\gamma(\underline{e}_i, z, \theta)$ ,  $i = 2, 3$ , given by (3.24)(3.25), do not depend on  $\theta$ , and the functions

$$\gamma(\underline{e}_1, z, \theta) = \frac{ie^{\frac{3\theta}{2}}}{h\sqrt{ze^{2\theta}}} 1_{(b, +\infty)} e^{i\frac{\sqrt{ze^{2\theta}}(x-b)}{h}}, \quad \gamma(\underline{e}_4, z, \theta) = \frac{ie^{\frac{3\theta}{2}}}{h\sqrt{ze^{2\theta}}} 1_{(-\infty, a)} e^{-i\frac{\sqrt{ze^{2\theta}}(x-a)}{h}}$$

are such that  $\forall f \in L^2(\mathbb{R})$ ,  $\theta \mapsto \langle f, \gamma(\underline{e}_i, z, \theta) \rangle_{L^2(\mathbb{R})}$  is analytic on  $S_\alpha$ . It follows that  $\theta \mapsto \gamma(\underline{e}_i, z, \theta)$  is a  $L^2(\mathbb{R})$ -valued analytic function on  $S_\alpha$ . This propriety holding for any  $z$  with  $\operatorname{Re} z < 0$ , we have also that  $\theta \mapsto \overline{\gamma(\underline{e}_i, \bar{z}, \bar{\theta})}$  is a  $L^2(\mathbb{R})$ -valued analytic function on  $S_\alpha$ . Therefore, for  $i, j = 1, \dots, 4$ , the operator with kernel  $\gamma(\underline{e}_i, z, \theta) \otimes \overline{\gamma(\underline{e}_j, \bar{z}, \bar{\theta})}$  is analytic w.r.t.  $\theta$  on the strip  $S_\alpha$ . It allows to conclude that  $\theta \mapsto (H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1}$  is a bounded operator-valued analytic map on the strip  $S_\alpha$ .  $\square$

## 3.2 Resonances

Next consider:  $H_{\theta_0, \mathcal{V}}^h = H_{\theta_0, 0}^h + \mathcal{V}$ , with  $\mathcal{V}$  fulfilling the assumptions (3.4). Local perturbations of  $H_{\theta_0, 0}^h$  can generate resonance poles for the associated resolvent operator. These can be detected through the deformation technique by means of an exterior complex scaling of the type introduced in (3.2). To fix this point, let us introduce the set of functions

$$\mathcal{A} = \left\{ u \mid u(x) = p(x)e^{-\beta x^2}, \beta > 0 \right\}, \quad (3.36)$$

where  $x \in \mathbb{R}$  and  $p$  is any polynomial. The action of  $U_\theta$  on the elements of  $\mathcal{A}$  is

$$U_\theta u(x) = \begin{cases} e^{\frac{\theta}{2}} p(e^\theta(x-b) + b) e^{-\beta(e^\theta(x-b)+b)^2}, & x > b \\ p(x) e^{-\beta x^2}, & x \in (a, b) \\ e^{\frac{\theta}{2}} p(e^\theta(x-a) + a) e^{-\beta(e^\theta(x-a)+a)^2}, & x < a. \end{cases} \quad (3.37)$$

If  $\operatorname{Re}(e^{2\theta} x^2) > \epsilon x^2$  for some  $\epsilon > 0$ , the function  $U_\theta u$  belongs to  $L^2(\mathbb{R})$ . In particular, for all positive  $\alpha < \frac{\pi}{4}$ , the map  $\theta \mapsto U_\theta u$  is a  $L^2$ -valued analytic map on the strip  $S_\alpha = \{\theta \in \mathbb{C} \mid |\operatorname{Im} \theta| \leq \alpha\}$ . According to the presentation of [32], the *quantum resonances* of  $H_{\theta_0, \mathcal{V}}^h$  are the poles of the meromorphic continuations of the function

$$z \mapsto F(z, 0) = \left\langle u, (H_{\theta_0, \mathcal{V}}^h - z)^{-1} v \right\rangle_{L^2(\mathbb{R})}, \quad u, v \in \mathcal{A}, \quad (3.38)$$

from  $\{z \in \mathbb{C}, \operatorname{Im} z > 0\}$  to  $\{z \in \mathbb{C}, \operatorname{Im} z < 0\}$ .

**Proposition 3.6.** *Let  $\theta_0 \in \mathbb{C}$  and  $u, v \in \mathcal{A}$ . Consider the map:  $z \mapsto F(z, 0)$ , a.e. defined in  $\{\mathbb{C} \mid \operatorname{Im} z > 0\}$ .*

1) *The map  $z \mapsto F(z, 0)$  has a meromorphic extension into the sector  $\{\arg z \in (-\frac{\pi}{2}, 0)\}$  of the*

second Riemann sheet.

2) The poles of the continuation of  $F(z, 0)$  into the cone

$$K_\tau = \{\arg z \in (-2\tau, 0)\}, \quad \text{with } \tau < \frac{\pi}{4},$$

are eigenvalues of the operators  $H_{\theta_0, \mathcal{V}}^h(\theta)$  with  $\tau \leq \text{Im } \theta < \frac{\pi}{4}$ .

**Proof:** 1) The proof adapts the ideas underlying the complex scaling method (see [23]) to the particular class exterior scaling maps  $U_\theta$ .

Consider the strip  $S_\alpha = \{\theta \in \mathbb{C} \mid |\text{Im } \theta| \leq \alpha\}$  for a positive  $\alpha < \frac{\pi}{4}$ . Then, consider the corresponding set  $\mathcal{O} \subset \mathbb{C}$  given in Proposition 3.5 and fix  $z \in \mathcal{O}$ . According to Proposition 3.5, and to the properties of  $U_\theta u$ ,  $u \in \mathcal{A}$ , the function

$$F(z, \theta) = \left\langle U_{\hat{\theta}} u, (H_{\theta_0, \mathcal{V}}^h(\theta) - z)^{-1} U_\theta v \right\rangle_{L^2(\mathbb{R})}$$

is analytic in the variable  $\theta \in S_\alpha$ . When  $\theta \in \mathbb{R}$ , the exterior scaling  $U_\theta$  is an unitary map and one has

$$F(z, \theta) = F(z, 0), \quad \forall \theta \in S_\alpha \cap \mathbb{R}.$$

Since  $F(z, \theta)$  is holomorphic in  $\theta$  and constant on the real line, this is a constant function in the whole strip  $S_\alpha$  and

$$F(z, \theta) = F(z, 0), \quad \forall \theta \in S_\alpha.$$

Now, fix  $\theta \in S_\alpha$  such that  $\text{Im } \theta > 0$ . It follows from Corollary 3.4 that  $\sigma_{ess}(H_{\theta_0, \mathcal{V}}^h(\theta)) = e^{-2i \text{Im } \theta} \mathbb{R}_+$  and the map  $z \mapsto F(z, \theta)$  is meromorphic on  $\mathbb{C} \setminus e^{-2i \text{Im } \theta} \mathbb{R}_+$  such that

$$F(z, \theta) = F(z, 0), \quad \forall z \in \mathcal{O}. \quad (3.39)$$

Since  $z \mapsto F(z, 0)$  is meromorphic on  $\mathbb{C} \setminus \mathbb{R}_+$ , the equality (3.39) holds as an identity of meromorphic functions  $\forall z$  with  $\text{Im } z > 0$ . We conclude that  $F(z, \theta)$  defines a meromorphic extension of  $F(z, 0)$  from the set  $\{z \in \mathbb{C} \mid \text{Im } z > 0\}$  to the sector  $\{\arg z \in (-2 \text{Im } \theta, 0)\}$ .

2) Consider  $0 < \tau < \frac{\pi}{4}$ . From the previous point, when  $\theta$  varies in  $\tau \leq \text{Im } \theta < \frac{\pi}{4}$ , the maps  $z \mapsto F(z, \theta)$  coincide in  $K_\tau$  with meromorphic extensions of  $F(z, 0)$ . Therefore, the poles of  $z \mapsto F(z, \theta)$  in  $K_\tau$  do not depend on  $\theta$  and correspond to the poles of the meromorphic extension of  $F(z, 0)$  in  $K_\tau$ . The vectors  $U_\theta u$ ,  $u \in \mathcal{A}$ , being dense in  $L^2(\mathbb{R})$ , the poles of  $z \mapsto F(z, \theta)$  corresponds to eigenvalues of  $H_{\theta_0, \mathcal{V}}^h(\theta)$ .  $\square$

### 3.3 A time dependent model

Consider the non-autonomous model  $H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)$ , where  $\mathcal{V}(t)$  is a family of self-adjoint potentials composed by  $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$

$$\mathcal{V}_1(t) \in C^0(\mathbb{R}_+; L^\infty((a, b))), \quad \mathcal{V}_2(t) = \sum_{j=1}^n \alpha_j(t) \delta(x - c_j), \quad (3.40)$$

with  $\{c_j\} \subset (a, b)$ ,  $\alpha_j(t) \in C^1(\mathbb{R}_+; \mathbb{R})$ . According to the specific feature of point perturbations, the domain's definition, given in (3.7), can be rephrased as

$$D(H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)) = \{u \in H^2(\mathbb{R} \setminus \{a, b, c_1, \dots, c_n\}) \cap H^1(\mathbb{R} \setminus \{a, b\}) \mid h^2 [u'(c_j^+) - u'(c_j^-)] = \alpha_j(t) u(c_j) \text{ and (3.6) holds}\}, \quad (3.41)$$

where time dependent boundary conditions appear in the interaction points  $c_j$ .

Most of the techniques employed in the analysis the Cauchy problem

$$\begin{cases} i \partial_t u = H(t) u \\ u_{t=0} = u_0 \end{cases} \quad (3.42)$$

for non-autonomous Hamiltonians,  $H(t)$ , require, as condition, that the operator's domain is independent of the time (we mainly refer to the Yoshida's and Kato's results ([36][37][61]); an extensive presentation of the subject can be found given in [26]). In the particular case of  $H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)$ , one can explicitly construct a family of unitary maps  $V_{t, t_0}$  such that

$$V_{t, t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t, t_0}^{-1} \quad (3.43)$$

has a constant domain. To fix this point, let us introduce a time dependent real vector field  $g(x, t)$  and assume

$$\begin{cases} \text{i) } g(\cdot, t) \in C^1(\mathbb{R}_+; C_0^\infty(\mathbb{R})), \\ \text{ii) } g(c_j, t) = 0, \quad j = 1, n, \quad \forall t, \\ \text{iii) } \text{supp } g(\cdot, t) = \cup_{j=1}^n I_{c_j}, \quad \text{with: } I_{c_j} = (c_j - \epsilon_j, c_j + \epsilon_j) \text{ and } \cap_j I_{c_j} = \emptyset. \end{cases} \quad (3.44)$$

For  $\epsilon_j$  small,  $g(\cdot, t)$  has support strictly included in  $(a, b)$  and localized around the interaction points  $x = c_j$ . According to i),  $g(\cdot, t)$  satisfy a global Lipschitz condition uniformly in time: then the dynamical system

$$\begin{cases} \dot{y}_t = g(y_t, t) \\ y_{t_0} = x \end{cases} \quad (3.45)$$

admits a unique global solution continuously depending on time and Cauchy data  $\{t_0, x\}$ . Using the notation:  $y_t = F(t, t_0, x)$ , one has

$$|F(t, t_0, x_1) - F(t, t_0, x_2)| \leq e^{M|t-t_0|} |x_1 - x_2|, \quad \text{with: } M = \sup_{x \in \mathbb{R}, t \geq 0} \partial_y g(y, t). \quad (3.46)$$

Consider the variations of  $F(t, t_0, x)$  w.r.t.  $x$ :  $z_t = \partial_x F(t, t_0, x)$ . From (3.45), one has

$$\begin{cases} \dot{z}_t = \partial_1 g(F(t, t_0, x), t) z_t \\ z_{t_0} = 1, \end{cases} \quad (3.47)$$

with  $\partial_1 g$  denoting the derivative w.r.t. the first variable. The solution to this problem is positive and explicitly given by

$$\partial_x F(t, t_0, x) = e^{\int_{t_0}^t \partial_1 g(F(s, t_0, x), s) ds} > 0 \quad \forall x \in \mathbb{R}. \quad (3.48)$$

According to (3.48),  $F(t, t_0, \cdot)$  is a  $C^\infty$ -diffeomorphism and the map  $x \mapsto F(t, t_0, x)$  is a time-dependent local dilation around the points  $c_j$ . In particular, it follows from the assumptions i) and ii) that

$$F(t, t_0, c_j) = c_j, \quad F(t, t_0, x) = x \text{ for all } x \in \mathbb{R} \setminus \text{supp } g, \quad (3.49)$$

and

$$F(t, t_0, F(t_0, \bar{t}, x)) = F(t, \bar{t}, x). \quad (3.50)$$

The unitary transformation associated with the change of variable  $x \rightarrow F(t, t_0, x)$  is

$$\begin{cases} (V_{t_0, t} u)(x) = (\partial_x F(t, t_0, x))^{\frac{1}{2}} u(F(t, t_0, x)) \\ V_{t, t_0} = V_{t_0, t}^{-1}. \end{cases} \quad (3.51)$$

Regarded as a function of time,  $t \mapsto V_{t_0, t}$  is a strongly continuous differentiable map and one has

$$\partial_t V_{t_0, t} = V_{t_0, t} \left[ \frac{1}{2} (\partial_y g) + g \partial_y \right]. \quad (3.52)$$

The form of the conjugated Hamiltonian  $V_{t, t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0, t}$  follows by direct computation

$$\begin{aligned} V_{t, t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0, t} &= -\hbar^2 \eta(y) [\partial_y b^2 \partial_y + (\partial_y a b) - a^2] \\ &\quad + \mathcal{V}_1(F(t_0, t, y), t) + \sum_{j=1}^n \alpha_j(t) b(c_j, t) \delta(x - c_j), \end{aligned} \quad (3.53)$$

$$b(y, t) = e^{\int_{t_0}^t \partial_1 g(F(s, t, y), s) ds}, \quad a(y, t) = \frac{1}{2} b^{\frac{1}{2}}(y, t) \int_{t_0}^t \partial_1^2 g(F(s, t, y), s) b(y, s) ds. \quad (3.54)$$

After conjugation, the boundary conditions in the operator's domain change as

$$h^2 b^2(c_j, t) [u'(c_j^+) - u'(c_j^-)] = b(c_j, t) \alpha_j(t) u(c_j). \quad (3.55)$$

Assume, for all  $j = 1 \dots n$

$$\text{iv) } \alpha_j(0) \neq 0; \quad \text{v) } \alpha_j(0) \alpha_j(t) > 0; \quad \text{vi) } \alpha_j(t) \in C^1(\mathbb{R}_+; \mathbb{R}). \quad (3.56)$$

One can determine (infinitely many)  $g(\cdot, t) \in C^0(\mathbb{R}_+; C_0^\infty(\mathbb{R}))$  such that

$$\partial_1 g(c_j, t) = \frac{\dot{\alpha}_j(t)}{\alpha_j(t)}. \quad (3.57)$$

This implies

$$b(c_j, t) = e^{\int_{t_0}^t \partial_1 g(F(s, t, c_j), s) ds} = e^{\int_{t_0}^t \partial_1 g(c_j, s) ds} = \frac{\alpha_j(t)}{\alpha_j(0)} \quad (3.58)$$

and (3.55) can be written in the time-independent form

$$h^2 [u'(c_j^+) - u'(c_j^-)] = \alpha_j(0) u(c_j). \quad (3.59)$$

Thus, the Hamiltonians  $V_{t, t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0, t}$  have common domain given by

$$Y = \{u \in H^2(\mathbb{R} \setminus \{a, b, c_j\}) \cap H^1(\mathbb{R} \setminus \{a, b\}) \mid [3.6], [3.59]\}. \quad (3.60)$$

Consider the time evolution problem for  $H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)$

$$\begin{cases} i \partial_t u = H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) u \\ u_{t_0} = u_0. \end{cases} \quad (3.61)$$

Setting  $v = V_{t, t_0} u$ , and

$$A(t) = V_{t, t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0, t} - i \left[ \frac{1}{2} (\partial_y g) + g \partial_y \right], \quad (3.62)$$

with  $D(A(t)) = Y$ , one has:  $v_{t_0} = u_{t_0}$ ,

$$\begin{cases} \partial_t v = -i A(t) v \\ v_{t_0} = u_0. \end{cases} \quad (3.63)$$

**Proposition 3.7.** *Let  $\mathcal{V}(t) = \mathcal{V}_1(t) + \mathcal{V}_2(t)$  be defined with the conditions (3.40) and (3.56). Assume:  $\theta = \theta_0 = i\tau$ , with  $\tau \in (0, \frac{\pi}{2})$ . There exists a unique family of operators  $U_{t, s}$ ,  $0 \leq s \leq t$ , with the following properties:*

**a)**  $U_{t, s}$  is strongly continuous in  $L^2(\mathbb{R})$  w.r.t. the variables  $s$  and  $t$  and fulfills the conditions:  $U_{s, s} = Id$ ,  $U_{t, s} \circ U_{s, r} = U_{t, r}$  for  $r \leq s \leq t$  and  $\|U_{t, s}\| \leq 1$  for any  $s$  and  $t$ ,  $s \leq t$ .

**b)** For  $u_s \in D(H_{\theta_0, \mathcal{V}(s)}^h(\theta_0))$ , one has:  $U_{t, s} u_s \in D(H_{\theta_0, \mathcal{V}(t)}^h(\theta_0))$  for all  $t \geq s$ . In particular, for fixed  $t$ ,  $U_{t, s}$  is strongly continuous w.r.t.  $s$  in the norm of  $H^2(\mathbb{R} \setminus \{a, b, c_j\}) \cap H^1(\mathbb{R} \setminus \{a, b\})$ . While, for fixed  $s$ ,  $U_{t, s}$  is strongly continuous w.r.t.  $t$  in the same norm, except possibly countable values of  $t \geq s$ .

**c)** For fixed  $s$  and  $u_s \in D(H_{\theta_0, \mathcal{V}(s)}^h(\theta_0))$ , the derivative  $\frac{d}{dt} U_{t, s} u_s$  exists and is strongly continuous in  $L^2(\mathbb{R})$  except, possibly, countable values  $t \geq s$ . With similar exceptions, one has:  $\frac{d}{dt} U_{t, s} u_s = -i H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) U_{t, s} u_s$ .

**d)** Additionally, if  $\mathcal{V}_1(t) \in C^1(\mathbb{R}_+, L^\infty((a, b))) \cap C^0(\mathbb{R}_+, W^{1, \infty}(\mathbb{R}))$ , and  $\alpha_j(t) \in C^2(\mathbb{R}_+; \mathbb{R})$ , then the conclusion of point (c) holds for all  $t \geq s$  without exceptions.

**Proof:** Since the Cauchy problems (3.61) and (3.63) are related by the time-differentiable map  $V_{t,t_0}$ , it is enough to prove the result in the case of  $A(t)$ . Let assume the conditions (3.44) and (3.58) to hold, and start to consider the properties of this operator.

I) As already noticed (see relation (3.11)),  $iH_{\theta_0, \mathcal{V}(t)}^h(\theta_0)$  is an accretive operator. This property extends to  $V_{t,t_0} \left( iH_{\theta_0, \mathcal{V}(t)}^h(\theta_0) \right) V_{t_0,t}$ , which is unitarily equivalent to an accretive operator, and to  $A(t)$ , since, as a straightforward computation shows, the contribution  $i \left[ \frac{1}{2} (\partial_y g) + g \partial_y \right]$  is self-adjoint. The spectral profile of  $A(t)$  essentially follows from the properties of  $H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)$ . Indeed, we notice that:  $\sigma \left( V_{t,t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0,t} \right) = \sigma \left( H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) \right)$ , since the two operators are unitarily equivalent. Moreover, the term  $i \left[ \frac{1}{2} (\partial_y g) + g \partial_y \right]$  is relatively compact w.r.t.  $V_{t,t_0} H_{\theta_0, \mathcal{V}(t)}^h(\theta_0) V_{t_0,t}$ , since it has a lower differential order (see definition (3.62)). Then,  $\sigma_{ess}(A(t)) = \sigma_{ess}(H_{\theta_0, \mathcal{V}(t)}^h(\theta_0)) = e^{-2i \operatorname{Im} \theta_0} \mathbb{R}_+$ , as it follows from Corollary 3.4, and  $(A(t) - z)^{-1}$  is a meromorphic function of  $z$  in  $\mathbb{C} \setminus e^{-2i \operatorname{Im} \theta_0} \mathbb{R}_+$ . This result yields:  $\sigma_{ess}(iA(t)) = e^{i(\frac{\pi}{2} - 2 \operatorname{Im} \theta_0)} \mathbb{R}_+$  and:  $\rho(iA(t)) \cap \mathbb{R}_- \neq \emptyset$ . As a consequence of the above, one has: i)  $iA(t)$  is accretive; 2)  $-\lambda_0 \in \rho(iA(t))$  for some  $\lambda_0 > 0$ . Then, for any fixed  $t$ ,  $iA(t)$  is the generator of a contraction semigroup,  $e^{-isA(t)}$ , on  $L^2(\mathbb{R})$  (see [51], Th. X.48). In particular, the operator's domain  $D(iA(t)) = Y$ , defined in (3.60), is invariant by the action of  $e^{-isA(t)} \implies Y$  is  $iA(t)$ -admissible for any  $t$ . Moreover, as  $iA(t)$  is the generator of a contraction semigroup, from the Hille-Yoshida's theorem it follows that

$$\begin{cases} \mathbb{R}_- \subset \rho(iA(t)), \\ \left\| (iA(t) + \lambda)^{-1} \right\| \leq \frac{1}{\lambda} \text{ for all } \lambda > 0. \end{cases} \quad (3.64)$$

In particular, for any finite collection of values  $0 \leq t_1 \leq \dots \leq t_k$ , one has

$$\left\| \prod_{j=1}^k (iA(t_j) + \lambda)^{-1} \right\| \leq \frac{1}{\lambda^k}. \quad (3.65)$$

This relation implies that  $iA(t)$  is *stable* (with coefficients  $M = 1$  and  $\beta = 0$ , according to the definition given in [37]).

II) Consider the action of  $A(t)$  on its domain. Here, the Hilbert space  $Y$  is provided with the norm  $H^2(\mathbb{R} \setminus \{a, b, c_1, \dots, c_n\}) \cap H^1(\mathbb{R} \setminus \{a, b\})$ . For  $u \in Y$ , we use the decomposition:  $u = 1_{\mathbb{R} \setminus (a,b)} u + 1_{(a,b)} u = u_{ext} + u_{in}$ . Recalling that the functions  $g(\cdot, t)$ ,  $b(\cdot, t)$ ,  $a(\cdot, t)$  are supported inside  $(a, b)$ , from the definition (3.53), (3.62), one has

$$(A(t) - A(s)) u = (A(t) - A(s)) u_{in}, \quad (3.66)$$

with

$$\begin{aligned} A(t) u_{in} &= \left[ -h^2 \partial_y b^2 \partial_y + \sum_{j=1}^n \alpha_j(t) b(c_j, t) \delta(x - c_j) \right] u_{in} \\ &+ \left[ -h^2 ((\partial_y a b) - a^2) + \mathcal{V}_1(F(t_0, t, y), t) - i \left( \frac{1}{2} (\partial_y g) + g \partial_y \right) \right] u_{in}. \end{aligned} \quad (3.67)$$

Taking into account the boundary conditions (3.59), the second order term in (3.67) writes as

$$-h^2 (\partial_y b^2 \partial_y) u_{in} = -h^2 (\partial_y b^2) \partial_y u_{in} - h^2 b^2 \Delta_{(a,b) \setminus \{c_j\}} u_{in} - \sum_{j=1}^n \alpha_j(0) b^2(c_j, t) u_{in}(c_j) \delta(x - c_j),$$

where, according to (3.58),

$$\sum_{j=1}^n \alpha_j(0) b^2(c_j, t) u_{in}(c_j) \delta(x - c_j) = \sum_{j=1}^n \alpha_j(t) b(c_j, t) u_{in}(c_j) \delta(x - c_j).$$

From these relations, it follows

$$\begin{aligned} A(t)u_{in} &= -h^2 b^2 \Delta_{(a,b) \setminus \{c_j\}} u_{in} - h^2 \left[ (\partial_y b^2) \partial_y + (\partial_y ab) - a^2 \right] u_{in} \\ &\quad + \mathcal{V}_1(F(t_0, t, y), t) u_{in} - i \left[ \frac{1}{2} (\partial_y g) + g \partial_y \right] u_{in}. \end{aligned}$$

Therefore, we have

$$\begin{aligned} (A(t) - A(s))u &= -h^2 \left[ (b_t^2 - b_s^2) \Delta_{(a,b) \setminus \{c_j\}} + (\partial_1 b_t^2 - \partial_1 b_s^2) \partial_y + (\partial_1 a_t b_t - \partial_1 a_s b_s) - (a_t^2 - a_s^2) \right] u_{in} \\ &\quad + (\mathcal{V}_1(F(t_0, t, y), t) - \mathcal{V}_1(F(t_0, s, y), s)) u_{in} - i \left[ \frac{1}{2} (\partial_1 g_t - \partial_1 g_s) + (g_t - g_s) \partial_y \right] u_{in}, \end{aligned}$$

and

$$\|(A(t) - A(s))u\|_{L^2(\mathbb{R})} \leq C_h M(t, s) \|u\|_{H^2(\mathbb{R} \setminus \{a, b, c_j\}) \cap H^1(\mathbb{R} \setminus \{a, b\})}, \quad (3.68)$$

where  $C_h$  is a positive constant depending on  $h$ , while

$$\begin{aligned} M(t, s) &= \|\mathcal{V}_1(t) - \mathcal{V}_1(s)\|_{L^\infty((a,b))} + \|a_t^2 - a_s^2\|_{C^0([a,b])} + \|\partial_1 a_t b_t - \partial_1 a_s b_s\|_{L^\infty((a,b))} \\ &\quad + \sum_{l=0,1} \left( \|\partial_1^l b_t^2 - \partial_1^l b_s^2\|_{L^\infty((a,b))} + \|\partial_1^l g_t - \partial_1^l g_s\|_{L^\infty((a,b))} \right). \end{aligned}$$

From our assumptions,  $t \mapsto g_t, b_t, a_t$  are continuous  $C^\infty$ -valued maps, and  $t \mapsto \mathcal{V}_1 \in C^0(\mathbb{R}_+, L^\infty)$ ; this yields:  $\lim_{s \rightarrow t} M(t, s) = 0$ , and, due to (3.68),

$$\lim_{s \rightarrow t} \|(A(t) - A(s))u\|_{L^2(\mathbb{R})} = 0, \quad \forall u \in Y.$$

This gives the continuity of  $t \mapsto A(t)$  in the  $\mathcal{L}(Y, L^2(\mathbb{R}))$ -operator norm.

III) Consider the map:  $S(t) = (iA(t) + \lambda_0)$  for  $\lambda_0 > 0$ . According to (3.64),  $S(t)$  defines a family of isomorphisms of  $Y$  to  $L^2(\mathbb{R})$ . Moreover, making use of the relations (3.53), (3.62) and the condition I3.58), the time derivative of  $S(t)$  writes as

$$\begin{aligned} \frac{d}{dt} S(t) &= -h^2 [\partial_y (2b \partial_t b) \partial_y + (\partial_{y,t} ab) - 2a \partial_t a] + \sum_{j=1}^n \frac{2\alpha_j(t) \alpha_j'(t)}{\alpha_j(0)} \delta(x - c_j) \\ &\quad + \partial_t \mathcal{V}_1(F(t_0, t, y), t) + (\partial_t F(t_0, t, y)) \partial_1 \mathcal{V}_1(F(t_0, t, y), t) - i \left[ \frac{1}{2} (\partial_{y,t} g) + (\partial_t g) \partial_y \right], \end{aligned}$$

where the term  $\partial_t F(t_0, t, y)$  can be written in the form

$$\partial_t F(t_0, t, y) = -b^{-1}(y, t) g(F(t_0, t, y), t),$$

as it follows by using:  $F(t, t_0, F(t_0, t, y)) = y$  and the definition of  $b(y, t)$ . Since the variations of the functions  $a, b, \mathcal{V}_1, g$  w.r.t. both the variables  $t$  and  $y$  are supported on  $(a, b)$ , each contribution to  $\frac{d}{dt} S(t)$  acts only inside this interval. Therefore,  $u \in D(\frac{d}{dt} S(t))$  is not expected to fulfill any interface condition at  $x = a, b$ , while in the interaction points  $c_j$ , one has

$$h^2 2b(c_j, t) \partial_t b(c_j, t) [u'(c_j^+) - u'(c_j^-)] = \frac{2\alpha_j(t) \alpha_j'(t)}{\alpha_j(0)} u(c_j),$$

which, according to (3.58), reduces to (3.59). It follows that:  $Y \subset D(\frac{d}{dt} S(t))$ , and one can consider the action of  $\frac{d}{dt} S(t)$  on  $Y$ . Proceeding as in point II and using the stronger assumptions:  $\mathcal{V}_1(t) \in C^1(\mathbb{R}_+, L^\infty((a, b))) \cap C^0(\mathbb{R}_+, W^{1,\infty}(\mathbb{R}))$ ,  $\alpha_j(t) \in C^2(\mathbb{R}_+; \mathbb{R})$ , one shows that  $\frac{d}{dt} S(t)$  is strongly continuous from  $Y$  to  $L^2(\mathbb{R})$ .

Finally, the points I and II resume as follows: i) the Hilbert space  $Y$  is  $A(t)$ -admissible for all  $t$ , ii)  $A(t)$  define a stable family operators  $t$ -continuous in the  $\mathcal{L}(Y, L^2(\mathbb{R}))$ -operator norm. Thus, the Theorem 5.2 in [37] applies and provides a strongly continuous dynamical system  $\mathcal{U}_{t,t_0}$ ,  $t_0 \leq t$ , for the Cauchy problem (3.63) with  $\|\mathcal{U}_{t,t_0}\| \leq 1$  and such that:

- 1) For fixed  $t_0$ , the family  $\mathcal{U}_{t,t_0}$  defines an a.e. strongly continuous flow in  $Y$ ; for fixed  $t$ ,  $\mathcal{U}_{t,t_0}$  is strongly continuous w.r.t.  $t_0$  in  $Y$ .
- 2) For  $y \in Y$ , the derivative  $\frac{d}{dt}\mathcal{U}_{t,t_0}y$  is a.e. strongly continuous in  $L^2(\mathbb{R})$  and one has:  $\frac{d}{dt}\mathcal{U}_{t,t_0}u_s = -iA(t)\mathcal{U}_{t,t_0}u_s$ . The conclusions (a), (b) and (c) of the statement follows by using the equivalence of the problems (3.61) and (3.63) through the maps  $V_{t,t_0}$ .

Moreover, assuming

$$\mathcal{V}_1(t) \in C^1(\mathbb{R}_+, L^\infty((a, b))) \cap C^0(\mathbb{R}_+, W^{1,\infty}(\mathbb{R})), \quad \alpha_j(t) \in C^2(\mathbb{R}_+; \mathbb{R})$$

it follows from point III that:  $S(t)$  is a family of isomorphisms from  $Y$  to  $L^2(\mathbb{R})$ , with

$$S(t)A(t)S^{-1}(t) = A(t)$$

and such that  $S(t)$  is strongly differentiable. In this case, Yoshida's Theorem applies (see Theorem 6.1 and Remark 6.2 in [37]) and the conclusion (d) of the statement follows.  $\square$

## 4 Exponential decay estimates

With this section, we start the analysis of the parameter dependent quantities as  $h \rightarrow 0$ . The exponential decay is specified with a good control of the prefactors which behave like  $\frac{1}{h^N}$ . These estimates are written for potentials with limited regularity assumptions in order to hold for the modelling of quantum wells in a semi-classical island with non-linear effect. Some preliminary estimates are reviewed in Appendix A.

### 4.1 Exponential decay for the Dirichlet problem

Consider  $V \in L^\infty((a, b); \mathbb{R})$ , and  $W^h = W_1^h + W_2^h$  an  $h$ -dependent real-valued potential with:

$$c1_{[a,b]} \leq V, \quad \|V\|_{L^\infty} \leq \frac{1}{c}, \quad \|W_1^h\|_{L^\infty} \leq \frac{1}{c}, \quad \|W_2^h\|_{\mathcal{M}_b} \leq \frac{1}{c}h, \quad (4.1)$$

where  $\|\mu\|_{\mathcal{M}_b}$  denotes the total variation of the measure  $\mu \in \mathcal{M}_b((a, b))$ . The constant  $c$  denotes a fixed positive value that can be chosen small when it is required by the analysis. We suppose that  $W_1^h$  and  $W_2^h$  are supported in the domain  $U_h = \{x \in (a, b); d(x, U) \leq h\}$  where  $U$  is a fixed compact subset of  $(a, b)$ .

After introducing the differential operators on  $(a, b)$

$$\tilde{P}^h := -h^2\Delta + V \quad \text{and} \quad P^h := -h^2\Delta + V - W^h,$$

two Dirichlet Hamiltonians are considered

$$\tilde{H}_D^h := -h^2\Delta + V = \tilde{P}^h, \quad \text{with} \quad D(\tilde{H}_D^h) = H^2((a, b)) \cap H_0^1((a, b)), \quad (4.2)$$

$$H_D^h := -h^2\Delta + V - W^h = P^h, \quad \text{with} \quad D(H_D^h) = \{u \in H_0^1((a, b)), P^h u \in L^2((a, b))\}. \quad (4.3)$$

For a real energy  $\lambda \in \mathbb{R}$  we consider the Agmon degenerate distance associated with  $V$

$$d_{Ag}(x, y, V, \lambda) = \int_x^y \sqrt{(V(t) - \lambda)_+} dt, \quad x \leq y.$$

And another tool that will be useful here is the  $h$ -dependent  $H^k$  norm

$$\|u\|_{H^{k,h}}^2 = \sum_{\alpha \leq k} \|(h\partial_x)^\alpha u\|_{L^2}^2. \quad (4.4)$$



**Proposition 4.1.** *i) Consider  $f = f_1 + f_2$  with  $f_1 \in L^2((a, b))$  and  $f_2 \in \mathcal{M}_b((a, b))$ . If  $V - \operatorname{Re} z \geq c$  with  $\|V\|_{L^\infty} \leq \frac{1}{c}$ , then any solution  $u \in H_0^1((a, b))$  to  $(\tilde{P}^h - z)u = f$  satisfies*

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|he^{\frac{\varphi}{h}} u'\|_{L^2} + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a,b,c}}{h} \left( \|f_1\|_{L^2} + \frac{1}{h^{\frac{1}{2}}} \|f_2\|_{\mathcal{M}_b} \right), \quad (4.5)$$

with  $\varphi(x) = d_{Ag}(x, K, V, \operatorname{Re} z)$  and  $K \supset \operatorname{supp} f_1 \cup \operatorname{supp} f_2$ .

*ii) Consider  $f \in L^2((a, b))$ . If  $V - \operatorname{Re} z \geq c$  with  $\|V\|_{L^\infty} \leq \frac{1}{c}$ , then any solution  $u \in D(H_D^h)$  to  $(H_D^h - z)u = f$  satisfies*

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|he^{\frac{\varphi}{h}} u'\|_{L^2} + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a,b,c}}{h} (\|u\|_{L^2} + \|f\|_{L^2}), \quad (4.6)$$

with  $\varphi(x) = d(x, K' \cup U, V, \operatorname{Re} z)$  and  $K' \supset \operatorname{supp} f$ . Especially when  $z \notin \sigma(H_D^h)$ , we have:

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|he^{\frac{\varphi}{h}} u'\|_{L^2} + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a,b,c}}{h} \left( \frac{1}{d(z, \sigma(H_D^h))} + 1 \right) \|f\|_{L^2},$$

and, when  $z = E^h$  is an eigenvalue of  $H_D^h$ , the related normalized eigenvector satisfies

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|he^{\frac{\varphi}{h}} u'\|_{L^2} + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a,b,c}}{h},$$

with  $\varphi(x) = d_{Ag}(x, U, V, E^h)$ .

**Remark 4.2.** The negative exponents of  $h$  in the upper bounds are not the optimal ones. Some care especially has to be taken while modifying  $\varphi$  or while commuting  $h\partial_x$  with  $e^{\frac{\varphi}{h}}$ . This presentation is the most flexible one for our purpose.

**Proof:** *i)* Our assumptions imply that the functions  $\varphi(x) = d_{Ag}(x, K, V, \operatorname{Re} z)$  and  $\varphi_h(x) = d_{Ag}(x, K_h, V - h, \operatorname{Re} z)$ , with  $K_h = \{x \in (a, b), d(x, K) \leq h\}$ , satisfy

$$|\varphi(x) - \varphi_h(x)| \leq \kappa_{a,b,c} h \quad \text{i.e.} \quad \left( \frac{e^{\frac{\varphi}{h}}}{e^{\frac{\varphi_h}{h}}} \right)^{\pm 1} \leq e^{\kappa_{a,b,c}},$$

for some uniform constant  $\kappa_{a,b,c}$ . Hence the function  $\varphi$  can be replaced by  $\varphi_h$  in the proof.

Lemma A.3 applied with  $\alpha = a$ ,  $\beta = b$ ,  $u_1 = u_2 = u$ ,  $\varphi = \varphi_h$  and  $v = e^{\frac{\varphi_h}{h}} u$  implies

$$\operatorname{Re} \int_a^b \bar{v} f \geq \int_a^b |hv'|^2 + \int_a^b h|v|^2.$$

Hence we get

$$\|v\|_{H^{1,h}}^2 \leq \frac{1}{h} (\|f_1\|_{L^2} \|v\|_{L^2} + \|f_2\|_{\mathcal{M}_b} \|v\|_{L^\infty}).$$

The Gagliardo-Nirenberg estimate  $\sup_{x \in [a, b]} |v(x)| \leq C_{b-a} \|v'\|_{L^2((a, b))}^{1/2} \|v\|_{L^2((a, b))}^{1/2}$  implies:

$$\|v\|_{H^{1,h}}^2 \leq \frac{1}{h} \left( \|f_1\|_{L^2} \|v\|_{H^{1,h}} + \frac{C_{b-a}}{h^{\frac{1}{2}}} \|f_2\|_{\mathcal{M}_b} \|v\|_{H^{1,h}} \right).$$

This combined with the equivalence of  $\|v\|_{H^{1,h}}$  with  $\|he^{\frac{\varphi_h}{h}} u'\|_{L^2} + \|u\|_{L^2}$  leads finally to (4.5).

*ii)* We follow the ideas of [24] which consists in putting the possibly negative term of the energy estimate in the left hand-side. Hence the equation  $(H_D^h - z)u = f$  is simply rewritten

$$(\tilde{H}_D^h - z)u = f + W_1^h u + W_2^h u,$$

and it suffices to estimate  $\|W_2^h u\|_{\mathcal{M}_b}$ . The Gagliardo-Nirenberg estimate gives

$$\|W_2^h u\|_{\mathcal{M}_b} \leq C_{b-a} \|W_2^h\|_{\mathcal{M}_b} \|u'\|_{L^2}^{1/2} \|u\|_{L^2}^{1/2}.$$

Applying Lemma A.3 with  $\alpha = a$ ,  $\beta = b$ ,  $u_1 = u_2 = u$ ,  $\varphi = 0$  leads to

$$\|hu'\|_{L^2}^2 + c\|u\|_{L^2}^2 \leq \left| \int_a^b f\bar{u} \right| + \left| \int_a^b W_1^h |u|^2 \right| + \left| \int_a^b W_2^h |u|^2 \right|.$$

Apply a second time the Gagliardo-Nirenberg estimate for

$$\|u\|_{H^{1,h}} \leq C_{a,b,c} \left( \|f\|_{L^2} + \|W_1^h\|_{L^\infty} \|u\|_{L^2} + \frac{1}{h} \|W_2^h\|_{\mathcal{M}_b} \|u\|_{L^2} \right)$$

gives

$$\|W_2^h u\|_{\mathcal{M}_b} \leq \frac{C'_{a,b,c}}{h^{\frac{1}{2}}} \|W_2^h\|_{\mathcal{M}_b} \left( \|f\|_{L^2} + \|W_1^h\|_{L^\infty} \|u\|_{L^2} + \frac{1}{h} \|W_2^h\|_{\mathcal{M}_b} \|u\|_{L^2} \right).$$

Combined with the results of **i)** applied with  $f$  replaced by  $f + W^h u$ , this yields:

$$\begin{aligned} h^{1/2} \sup_{x \in [a,b]} |e^{\frac{\varphi_h(x)}{h}} u(x)| + \|he^{\frac{\varphi_h}{h}} u'\|_{L^2} + \|e^{\frac{\varphi_h}{h}} u\|_{L^2} &\leq \frac{C''_{a,b,c}}{h} (\|f\|_{L^2} + \|W_1^h\|_{L^\infty} \|u\|_{L^2} \\ &\quad + \frac{1}{h} \|W_2^h\|_{\mathcal{M}_b} \|f\|_{L^2} + \frac{1}{h} \|W_2^h\|_{\mathcal{M}_b} \|W_1^h\|_{L^\infty} \|u\|_{L^2} + \frac{1}{h^2} \|W_2^h\|_{\mathcal{M}_b}^2 \|u\|_{L^2}), \end{aligned}$$

where  $\varphi_h(x) = d_{Ag}(x, K_h, V, \text{Re } z)$  and  $K_h = \{x \in (a, b), d(x, K' \cup U) < h\}$ . With the assumptions on  $W_1^h$  and  $W_2^h$  and replacing  $\varphi_h(x)$  by  $\varphi(x) = d_{Ag}(x, K' \cup U, V, \text{Re } z)$ , we obtain (4.6).  $\square$

## 4.2 Reduced boundary problem for generalized eigenfunctions

We shall consider the boundary value problem

$$\begin{cases} (\tilde{P}^h - z)u = f, \\ [h\partial_x + i\zeta^{1/2}]u(a) = \ell_a, \\ [h\partial_x - i\zeta^{1/2}]u(b) = \ell_b, \end{cases} \quad (4.7)$$

with  $\text{Im } z$  and  $\text{Im } \zeta$  small enough w.r.t  $h > 0$  and specified later. Here  $z^{1/2}$  denotes the complex square root with the determination  $\arg z \in [-\frac{\pi}{2}, \frac{3\pi}{2})$ .

The case  $f \equiv 0$  occurs while studying the generalized eigenfunctions of  $H_{V,\theta_0}(0)$  or their variation w.r.t  $\theta_0$ . The case  $\ell_a = \ell_b = 0$  is concerned with the resolvent estimates for the non self-adjoint Hamiltonians

$$\begin{aligned} \tilde{H}_\zeta^h &:= \tilde{P}^h, \text{ with } D(\tilde{H}_\zeta^h) = \{u \in H^2((a, b)), [h\partial_x + i\zeta^{1/2}]u(a) = 0, \\ &\quad [h\partial_x - i\zeta^{1/2}]u(b) = 0\}, \end{aligned} \quad (4.8)$$

$$\begin{aligned} H_\zeta^h &:= P^h, \text{ with } D(H_\zeta^h) = \{u \in H^1((a, b)), P^h u \in L^2((a, b)), \\ &\quad [h\partial_x + i\zeta^{1/2}]u(a) = 0, [h\partial_x - i\zeta^{1/2}]u(b) = 0\}. \end{aligned} \quad (4.9)$$

**Lemma 4.3.** *Assume  $V - \text{Re } z \geq c$  with  $\|V\|_{L^\infty} \leq \frac{1}{c}$  and  $|\text{Im } \zeta^{1/2}| \leq \frac{h}{\kappa_{b-a}}$  for  $\kappa_{b-a}$  large enough according to  $b - a$ . Let  $K$  be a compact subset of  $[a, b]$  and set  $\varphi = d_{Ag}(x, K, V, \text{Re } z)$ . Then any solution  $u \in L^2((a, b))$  to the boundary value problem (4.7) with  $f \equiv 0$  satisfies:*

$$h^{1/2} \sup_{x \in [a,b]} |e^{\pm \frac{\varphi(x)}{h}} u(x)| + \|he^{\pm \frac{\varphi}{h}} u'\|_{L^2} + \|e^{\pm \frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a,b,c}}{h^{1/2}} [|\ell_a| e^{\pm \frac{\varphi(a)}{h}} + |\ell_b| e^{\pm \frac{\varphi(b)}{h}}].$$

**Proof:** Again the function  $\varphi$  is replaced by  $\varphi_h(x) = d_{Ag}(x, K, V - h, \text{Re } z)$ . Applying Lemma A.3 with  $\alpha = a$ ,  $\beta = b$ ,  $u_1 = u_2 = u$  and  $v = e^{\frac{\varphi_h}{h}} u$  implies

$$\begin{aligned} 0 \geq \int_a^b |hv'|^2 + \int_a^b h|v|^2 + h \text{Re } (-i\zeta^{1/2}) [|v|^2(a) + |v|^2(b)] \\ + h \text{Re } \left[ \overline{v(a)} (e^{\pm \frac{\varphi_h(a)}{h}} \ell_a) - \overline{v(b)} (e^{\pm \frac{\varphi_h(b)}{h}} \ell_b) \right]. \end{aligned}$$

With the Gagliardo-Nirenberg estimate, we get

$$\|hv'\|_{L^2}^2 + h\|v\|_{L^2}^2 - 2C_{b-a}^2 |\operatorname{Im} \zeta^{1/2}| \|hv'\|_{L^2} \|v\|_{L^2} \leq C_{b-a} \|hv'\|_{L^2}^{1/2} \|v\|_{L^2}^{1/2} h^{1/2} \left[ e^{\pm \frac{\varphi_h(a)}{h}} |\ell_a| + e^{\pm \frac{\varphi_h(b)}{h}} |\ell_b| \right],$$

which implies

$$(\|hv'\|_{L^2}^2 + \|v\|_{L^2}^2)^{1/2} \leq \frac{C_{a,b,c}}{h^{1/2}} \left[ e^{\pm \frac{\varphi_h(a)}{h}} |\ell_a| + e^{\pm \frac{\varphi_h(b)}{h}} |\ell_b| \right],$$

provided  $\kappa_{b-a}$  is large enough according to the Gagliardo-Nirenberg constant  $C_{b-a}$ . Rewriting the inequality with the uniform equivalence  $\|he^{\pm \frac{\varphi_h}{h}} u'\|_{L^2} + \|e^{\pm \frac{\varphi_h}{h}} u\|_{L^2}$  with  $\|v\|_{H^{1,h}} = (\|hv'\|_{L^2}^2 + \|v\|_{L^2}^2)^{1/2}$  yields the result.  $\square$

The generalized eigenfunction  $\tilde{\psi}_{-, \theta_0}^h(k, x)$ ,  $k \in \mathbb{R}^*$ , of  $H_{V, \theta_0}^h(0)$  is the solution to

$$\begin{aligned} (\tilde{P}^h - k^2)\psi &= 0 \quad \text{in } \mathbb{R} \setminus \{a, b\} \\ \psi(a^+) &= e^{-\frac{\theta_0}{2}} \psi(a^-) \quad , \quad \psi'(a^+) = e^{-\frac{3\theta_0}{2}} \psi'(a^-) \\ \psi(b^-) &= e^{-\frac{\theta_0}{2}} \psi(b^+) \quad , \quad \psi'(b^-) = e^{-\frac{3\theta_0}{2}} \psi'(b^+) \\ \psi|_{(-\infty, a)} &= e^{i\frac{kx}{h}} + R(k)e^{-i\frac{kx}{h}} \quad , \quad \psi|_{(b, +\infty)} = T(k)e^{i\frac{kx}{h}} \quad \text{for } k > 0 \\ \psi|_{(-\infty, a)} &= T(k)e^{i\frac{kx}{h}} \quad , \quad \psi|_{(b, +\infty)} = e^{i\frac{kx}{h}} + R(k)e^{-i\frac{kx}{h}} \quad \text{for } k < 0. \end{aligned}$$

This can be reformulated as the boundary value problem in  $(a, b)$

$$\left\{ \begin{array}{ll} (\tilde{P}^h - k^2)\psi = 0 & \text{in } (a, b), \\ \left[ h\partial_x + i(k^2)^{1/2} e^{-\theta_0} \right] \psi(a) = & \begin{array}{l} (k > 0) \\ 2ike^{-\frac{3\theta_0}{2}} e^{i\frac{ka}{h}} \end{array} \\ \left[ h\partial_x - i(k^2)^{1/2} e^{-\theta_0} \right] \psi(b) = & \begin{array}{l} (k < 0) \\ 0, \\ 2ike^{-\frac{3\theta_0}{2}} e^{i\frac{kb}{h}}, \end{array} \end{array} \right. \quad (4.10)$$

where the choice of  $z^{1/2}$  says  $(k^2)^{1/2} = |k|$  for  $k \in \mathbb{R}^*$ . A straightforward application of Lemma 4.3 gives the next result.

**Proposition 4.4.** *Assume  $V - k^2 \geq c$ ,  $\|V\|_{L^\infty} \leq \frac{1}{c}$  and  $|\theta_0| \leq ch$  for  $c$  small enough according to  $a, b$ . The generalized eigenfunction  $\tilde{\psi}_{-, \theta_0}^h(k, \cdot)$  satisfies*

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} \tilde{\psi}_{-, \theta_0}^h(k, x)| + \|he^{\frac{\varphi}{h}} \tilde{\psi}_{-, \theta_0}^h(k, \cdot)'\|_{L^2} + \|e^{\frac{\varphi}{h}} \tilde{\psi}_{-, \theta_0}^h(k, \cdot)\|_{L^2} \leq \frac{C_{a,b,c}}{h^{1/2}},$$

$$\begin{aligned} \text{with} \quad \varphi(x) &= d_{Ag}(x, a, V, k^2) \quad \text{when } k > 0, \\ \text{and with} \quad \varphi(x) &= d_{Ag}(x, b, V, k^2) \quad \text{when } k < 0. \end{aligned}$$

With this first a priori estimate, the boundary value problem (4.10) can be rewritten

$$\left\{ \begin{array}{ll} (\tilde{P}^h - k^2)\psi = 0 & \text{in } (a, b), \\ \left[ h\partial_x + i(k^2)^{1/2} \right] \psi(a) = & \begin{array}{l} (k > 0) \\ 2ike^{i\frac{ka}{h}} + \mathcal{O}(\frac{|\theta_0|}{h}) \end{array} \\ \left[ h\partial_x - i(k^2)^{1/2} \right] \psi(b) = & \begin{array}{l} (k < 0) \\ \mathcal{O}(\frac{e^{-\frac{d_{Ag}(a,b,V,k^2)}{h}} |\theta_0|}{h}) \\ 2ike^{i\frac{kb}{h}} + \mathcal{O}(\frac{|\theta_0|}{h}). \end{array} \end{array} \right.$$

Hence the difference  $u = \tilde{\psi}_{-, \theta_0}^h - \tilde{\psi}_{-, 0}^h$  solves the boundary value problem

$$\left\{ \begin{array}{ll} (\tilde{P}^h - k^2)u = 0 & \text{in } (a, b), \\ \left[ h\partial_x + i(k^2)^{1/2} \right] u(a) = & \begin{array}{l} (k > 0) \\ \mathcal{O}(\frac{|\theta_0|}{h}) \end{array} \\ \left[ h\partial_x - i(k^2)^{1/2} \right] u(b) = & \begin{array}{l} (k < 0) \\ \mathcal{O}(\frac{e^{-\frac{d_{Ag}(a,b,V,k^2)}{h}} |\theta_0|}{h}) \\ \mathcal{O}(\frac{|\theta_0|}{h}). \end{array} \end{array} \right.$$

Hence Lemma 4.3 yields the next comparison result.

**Proposition 4.5.** Assume  $V - k^2 \geq c$ ,  $\|V\|_{L^\infty} \leq \frac{1}{c}$  and  $|\theta_0| \leq ch$  for  $c$  small enough according to  $a, b$ . The difference of generalized eigenfunctions  $u = \tilde{\psi}_{-, \theta_0}^h(k, \cdot) - \tilde{\psi}_{-, 0}^h(k, \cdot)$  satisfies

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|he^{\frac{\varphi}{h}} u'\|_{L^2} + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a, b, c} |\theta_0|}{h^{3/2}},$$

$$\text{with } \varphi(x) = d_{Ag}(x, a, V, k^2) \quad \text{when } k > 0,$$

$$\text{and with } \varphi(x) = d_{Ag}(x, b, V, k^2) \quad \text{when } k < 0.$$

**Remark 4.6.** With an additional regularity assumption [46] proves in the case  $\theta_0 = 0$  that the upper bound of  $\sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} \tilde{\psi}_{-, 0}^h(k, x)|$  is actually  $\mathcal{O}(1)$  with a first order WKB approximation. By using this result and the comparison result of Proposition 4.5 with a bootstrap argument or reconsidering the complete proof of [46], the estimate  $\sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} \tilde{\psi}_{-, 0}^h(k, x)| = \mathcal{O}(1)$  and  $\sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} (\tilde{\psi}_{-, \theta_0}^h - \tilde{\psi}_{-, 0}^h)(k, x)| = \mathcal{O}(\frac{|\theta_0|}{h^{1/2}})$  could be obtained. Here only  $V \in L^\infty$  is assumed with a possible loss in the  $h$ -exponent.

### 4.3 Weighted resolvent estimates

We complete the analysis of the previous subsection with results concerned with the resolvent  $(\tilde{H}_\zeta^h - z)^{-1}$  corresponding to the boundary value problem (4.7) with  $\ell_a = \ell_b = 0$ .

**Proposition 4.7.** Assume  $V - \operatorname{Re} z \geq c$ ,  $\|V\|_{L^\infty} \leq \frac{1}{c}$  and  $|\operatorname{Im} \zeta^{1/2}| \leq \frac{h}{\kappa_{b-a}}$  with  $\kappa_{b-a}$  large enough according to  $b - a$ . Let  $K$  be a compact subset of  $[a, b]$  and set  $\varphi = d_{Ag}(x, K, V, \operatorname{Re} z)$ . Then for  $f \in L^2((a, b))$ , the function  $u = (\tilde{H}_\zeta^h - z)^{-1} f$  satisfies

$$h^{1/2} \sup_{x \in [a, b]} |e^{\pm \frac{\varphi(x)}{h}} u(x)| + \|he^{\pm \frac{\varphi}{h}} u'\|_{L^2} + \|e^{\pm \frac{\varphi}{h}} u\|_{L^2} \leq \frac{C_{a, b, c}}{h} \|e^{\pm \frac{\varphi}{h}} f\|_{L^2},$$

where  $e^{\pm \frac{\varphi}{h}} f = f$  when  $\operatorname{supp} f \subset K$ .

In particular this yields

$$\left\| e^{\pm \frac{\varphi}{h}} (\tilde{H}_\zeta^h - z)^{-1} e^{\mp \frac{\varphi}{h}} \right\|_{\mathcal{L}(L^2)} \leq \frac{C_{a, b, c}}{h},$$

and  $z \in \rho(\tilde{H}_\zeta^h)$ .

**Proof:** Again we can replace  $\varphi$  by  $\varphi_h = d_{Ag}(x, K, V - h, \operatorname{Re} z)$ . Lemma A.3 with  $v = e^{\pm \frac{\varphi_h}{h}} u$  implies

$$\int_a^b |hv'|^2 + h \int_a^b |v|^2 + h \operatorname{Re} (-i\zeta^{1/2}) [|v(a)|^2 + |v(b)|^2] \leq \|e^{\pm \frac{\varphi_h}{h}} f\|_{L^2} \|v\|_{L^2}.$$

Absorbing the boundary term with the help of the Gagliardo-Nirenberg inequality like in the proof of Lemma 4.3 and taking  $\kappa_{b-a}$  large enough yields the result.  $\square$

**Proposition 4.8.** Assume  $V - \operatorname{Re} z \geq c$ ,  $\|V\|_{L^\infty} \leq \frac{1}{c}$ ,  $|\operatorname{Im} z^{1/2}| \leq \frac{h}{\kappa_{b-a}}$  and  $|\operatorname{Im} \zeta^{1/2}| \leq \frac{h}{\kappa_{b-a}}$  with  $\kappa_{b-a}$  large enough according to  $b - a$ . Let  $K$  be a compact subset of  $[a, b]$  and set  $\varphi = d_{Ag}(x, K, V, \operatorname{Re} z)$ . Then for  $f \in L^2((a, b))$ , the difference  $w = (\tilde{H}_z^h - z)^{-1} f - (\tilde{H}_\zeta^h - z)^{-1} f$  satisfies

$$h^{1/2} \sup_{x \in [a, b]} |e^{\pm \frac{\varphi(x)}{h}} w(x)| + \|he^{\pm \frac{\varphi}{h}} w'\|_{L^2} + \|e^{\pm \frac{\varphi}{h}} w\|_{L^2} \leq \frac{C_{a, b, c} |z^{1/2} - \zeta^{1/2}|}{h^2} \|e^{\pm \frac{\varphi}{h}} f\|_{L^2},$$

where  $e^{\pm \frac{\varphi}{h}} f = f$  when  $\operatorname{supp} f \subset K$ .

In particular this yields

$$\left\| e^{\pm \frac{\varphi}{h}} \left[ (\tilde{H}_z^h - z)^{-1} - (\tilde{H}_\zeta^h - z)^{-1} \right] e^{\mp \frac{\varphi}{h}} \right\|_{\mathcal{L}(L^2)} \leq \frac{C_{a, b, c} |z^{1/2} - \zeta^{1/2}|}{h^2}.$$

**Proof:** The function  $(\tilde{H}_\zeta^h - z)^{-1}f$  solves (4.7) with  $\ell_a = \ell_b = 0$ . Therefore, if we set  $u = (\tilde{H}_z^h - z)^{-1}f$  and  $v = (\tilde{H}_\zeta^h - z)^{-1}f$ , the function  $w = u - v$  verifies:

$$\begin{cases} (\tilde{P}^h - z)w = 0, \\ \begin{bmatrix} h\partial_x + iz^{1/2} \\ h\partial_x - iz^{1/2} \end{bmatrix} w(a) = -i(z^{1/2} - \zeta^{1/2})v(a), \\ \begin{bmatrix} h\partial_x + iz^{1/2} \\ h\partial_x - iz^{1/2} \end{bmatrix} w(b) = i(z^{1/2} - \zeta^{1/2})v(b). \end{cases}$$

Then it follows from Lemma 4.3 that:

$$h^{1/2} \sup_{x \in [a,b]} |e^{\pm \frac{\varphi(x)}{h}} w(x)| + \|he^{\pm \frac{\varphi}{h}} w'\|_{L^2} + \|e^{\pm \frac{\varphi}{h}} w\|_{L^2} \leq \frac{C_{a,b,c}}{h} |z^{1/2} - \zeta^{1/2}| 2h^{1/2} \sup_{x \in [a,b]} |e^{\pm \frac{\varphi(x)}{h}} v(x)|,$$

and we can apply Proposition 4.7 to the function  $v$  to get the result.  $\square$

## 5 Accurate analysis of resonances

In this section, we use the approach of Helffer-Sjöstrand relying on the introduction of a Grushin problem (see [30][56]). This section ends with a rewriting of the Fermi Golden rule (1.2) for the modified Hamiltonian  $H_{\theta_0, V-W^h}^h$ .

### 5.1 Resonances

Resonances for  $H_{\theta_0, V-W^h}^h = H_{\theta_0, V-W^h}^h(0)$  are eigenvalues of  $H_{\theta_0, V-W^h}^h(i\tau)$  for a suitable choice of  $\tau$  according to the resonances to be revealed. Associated eigenfunctions are the  $g_r \in L^2(\mathbb{R})$  functions satisfying

$$H_{\theta_0, V-W^h}^h(i\tau)g_r = z_r g_r, \quad (5.1)$$

with  $\arg(z_r) \in (-2\tau, 0)$ . Alternatively,  $f_r = U_{-i\tau}g_r$  satisfies

$$H_{\theta_0, V-W^h}^h f_r = z_r f_r,$$

with  $f_r \in L^2((a + e^{i\tau}\mathbb{R}_-) \cup (a, b) \cup (b + e^{i\tau}\mathbb{R}_+))$ . We refer to [29] for a general comparison of the two approaches. Accordingly, we recover the definition of Gamow resonant functions with no incoming data and slowly exponentially increasing outgoing waves.

Equivalently working with  $g_r$ , the condition  $g_r \in L^2(\mathbb{R})$  imposes the exponential modes in the exterior domain:

$$g_r(x) = \begin{cases} g_+ e^{i \frac{z_r^{1/2} e^{i\tau}}{h} (x-b)}, & x > b \\ g_{r,int}(x), & x \in (a, b) \\ g_- e^{-i \frac{z_r^{1/2} e^{i\tau}}{h} (x-a)}, & x < a, \end{cases} \quad (5.2)$$

where we recall that  $z^{1/2}$  denotes the complex square root with the determination  $\arg z \in [-\frac{\pi}{2}, \frac{3\pi}{2})$ . According to the definition of  $D(H_{\theta_0, V-W^h}^h(\theta))$ , this function verifies the following boundary conditions

$$(h\partial_x - iz_r^{1/2} e^{i\tau})g_r(b^+) = 0 \Rightarrow (h\partial_x - iz_r^{1/2} e^{-\theta_0})g_r(b^-) = 0,$$

and

$$(h\partial_x + iz_r^{1/2} e^{i\tau})g_r(a^-) = 0 \Rightarrow (h\partial_x + iz_r^{1/2} e^{-\theta_0})g_r(a^+) = 0$$

(with  $(z_r e^{-2\theta_0})^{1/2} = z_r^{1/2} e^{-\theta_0}$ ). It follows that the interior part of the solution satisfies the non-linear eigenvalue problem

$$H_{z_r e^{-2\theta_0}}^h g_{r,int} = z_r g_{r,int} \quad (5.3)$$

(see definition (4.9)). Conversely, given  $z_r$  in the sector:  $\arg(z_r) \in (-2\tau, 0)$  for which  $g_{r,int}$  fulfilling (5.3), it is possible to define suitable coefficients  $g_+$  and  $g_-$  such that the function  $g_r$  given by (5.2) is in  $D(H_{\theta_0, V-W^h}^h(\theta))$  and solves the equation (5.1). This allows to identify resonances with the

poles of  $(H_{ze^{-2\theta_0}}^h - z)^{-1}$ .

It is worthwhile to notice that this technique extends to the first Riemann sheet: in this case the poles of  $(H_{ze^{-2\theta_0}}^h - z)^{-1}$  correspond to proper eigenvalues of  $H_{\theta_0, V-W^h}^h$  provided that  $\arg(z) \leq \frac{3\pi}{2} - 2\tau$ . To this concern, the following spectral characterization holds.

**Lemma 5.1.** *Let  $H_{i\tau, V-W^h}^h(0)$  be defined as in (3.3) with  $\tau \in (0, \frac{\pi}{4})$ , then*

$$\sigma_p(H_{i\tau, V-W^h}^h(0)) \cap \{\operatorname{Im} z > 0\} = \emptyset.$$

**Proof:** According to the Proposition 3.6, the points in  $\sigma_p(H_{\theta_0, V-W^h}^h(0)) \cap \{\operatorname{Im} z > 0\}$  coincides with the eigenvalues of  $H_{\theta_0, V-W^h}^h(\theta)$ , in  $\operatorname{Im} z > 0$ , for any choice of  $\theta$  with:  $\operatorname{Im} \theta \in (0, \frac{\pi}{4})$ . In particular, for  $\theta = \theta_0 = i\tau$ , it follows from (3.11) that the operator  $H_{i\tau, V-W^h}^h(i\tau)$  is accretive. In this case,  $\sigma_p(H_{i\tau, V-W^h}^h(i\tau)) \cap \{\operatorname{Im} z > 0\} = \emptyset$ .  $\square$

## 5.2 The Grushin problem for resonances

In the previous section we got some accurate estimates for the variation w.r.t  $\theta_0$  of the generalized eigenfunctions of the filled well Hamiltonian  $H_{\theta_0, V}^h$ . Here the resonances for the full Hamiltonians  $H_{\theta_0, V-W^h}^h$  and  $H_{0, V-W^h}^h$  are considered. After reducing the problem to the interval  $[a, b]$ , we introduce like in [30][20][21] the Grushin problem modelled from the Dirichlet operator with the potential  $V - W^h$  for the boundary value operator  $H_\zeta^h - z$  with  $\zeta = z$  or  $\zeta = ze^{-2\theta_0}$  according to (4.9).

We assume that a cluster of eigenvalues  $\lambda_1^h, \dots, \lambda_\ell^h$  of the Dirichlet operator

$$H_D^h = -h^2 \Delta + V - W^h$$

exists such that

$$d(\lambda^0, \sigma(H_D^h) \setminus \{\lambda_1^h, \dots, \lambda_\ell^h\}) \geq c, \quad (5.4)$$

$$c \leq \lambda^0 \leq \inf_{x \in (a, b)} V(x) - c \leq \|V\|_{L^\infty} \leq \frac{1}{c}, \quad (5.5)$$

$$\max_{1 \leq j \leq \ell} |\lambda_j^h - \lambda^0| \leq \frac{1}{c} h. \quad (5.6)$$

The domain  $\omega_{ch}$  will be a neighborhood of  $\{\lambda_1^h, \dots, \lambda_\ell^h\}$  such that

$$\omega_{ch} \subset \{z \in \mathbb{C}, d(z, \{\lambda_1^h, \dots, \lambda_\ell^h\}) \leq ch\}. \quad (5.7)$$

**Remark 5.2.** *Notice that these assumptions do not forbid  $h$ -dependent  $\lambda^0$  with  $|\lambda^0(h) - \lambda^0| \leq \frac{1}{c} h$  since, in this case, it suffices to replace  $V$  by  $V - \lambda^0(h) + \lambda^0$ .*

Normalized eigenvectors associated with the  $\lambda_j^h$  are denoted by  $\Phi_j^h$  and the total spectral projector is

$$\Pi^h = \sum_{j=1}^{\ell} |\Phi_j^h\rangle \langle \Phi_j^h|.$$

We also introduce the bounded operators

$$R_0^- : \mathbb{C}^\ell \rightarrow L^2((a, b))$$

$$u^- = \begin{pmatrix} u_1 \\ \vdots \\ u_\ell \end{pmatrix} \mapsto R_0^- u^- = \sum_{j=1}^{\ell} u_j \Phi_j^h,$$

$$\text{and } R_0^+ : L^2((a, b)) \rightarrow \mathbb{C}^\ell$$

$$u \mapsto R_0^+ u = \begin{pmatrix} \langle \Phi_1^h, u \rangle \\ \vdots \\ \langle \Phi_\ell^h, u \rangle \end{pmatrix}.$$

For  $z \in \omega_{ch}$ , the matricial operator  $\begin{pmatrix} H_D^h - z & R_0^- \\ R_0^+ & 0 \end{pmatrix} : D(H_D^h) \times \mathbb{C}^\ell \rightarrow L^2((a, b)) \times \mathbb{C}^\ell$  is invertible with the inverse

$$\begin{pmatrix} H_D^h - z & R_0^- \\ R_0^+ & 0 \end{pmatrix}^{-1} = \begin{pmatrix} E_0(z) & E_0^+ \\ E_0^- & E_0^{-+}(z) \end{pmatrix},$$

$$E_0(z) = (H_D^h - z)^{-1}(1 - \Pi^h), \quad E_0^+ v^+ = \sum_{j=1}^{\ell} v_j \Phi_j^h,$$

$$E_0^- v = \begin{pmatrix} \langle \Phi_1^h, v \rangle \\ \vdots \\ \langle \Phi_\ell^h, v \rangle \end{pmatrix}, \quad E_0^{-+}(z) v^+ = \text{diag}(z - \lambda_j^h) v^+.$$

**Notations:** We set

$$\mathcal{H}_D(z) = \begin{pmatrix} H_D^h - z & R_0^- \\ R_0^+ & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{E}_D(z) = \begin{pmatrix} E_0(z) & E_0^+ \\ E_0^- & E_0^{-+}(z) \end{pmatrix}.$$

The problem  $(H_\zeta^h - z)u = f$  is studied after introducing the matricial operator

$$\mathcal{H}_\zeta(z) := \begin{pmatrix} H_\zeta^h - z & \chi_h R_0^- \\ R_0^+ & 0 \end{pmatrix}, \quad (5.8)$$

where the function  $\chi_h \in \mathcal{C}_0^\infty((a, b))$  satisfies

$$\|(h\partial_x)^\alpha \chi_h\|_{L^\infty((a, b))} \leq C_\alpha, \quad \alpha \in \mathbb{N} \quad \text{and} \quad \chi_h(x) \equiv 1 \text{ if } d(x, \{a, b\}) \geq h.$$

Another cut-off function  $\psi \in \mathcal{C}_0^\infty((a, b))$  will be used with a smaller support. By introducing the positive quantity

$$S_0 := d_{Ag}(\{a, b\}, U, V, \lambda^0),$$

the cut-off  $\psi$  is chosen such that for some  $\eta > 0$  independent of  $h > 0$  but to be specified later

$$\psi(x) = \begin{cases} 0 & \text{if } d_{Ag}(x, U, V, \lambda^0) > \frac{S_0 + \eta}{2} \\ 1 & \text{if } d_{Ag}(x, U, V, \lambda^0) < \frac{S_0 - \eta}{2}. \end{cases}$$

When  $\eta > 0$  and  $h > 0$  are small enough

$$U \subset \subset \{\psi \equiv 1\} \subset \text{supp } \psi \subset \subset \{\chi_h \equiv 1\}.$$

For  $z, \zeta \in \omega_{ch}$ , consider the approximate inverse

$$\mathcal{F}_\zeta(z) = \begin{pmatrix} \chi_h E_0 \psi + (1 - \rho_h)(\tilde{H}_\zeta^h - z)^{-1}(1 - \psi) & \chi_h E_0^+ \\ E_0^- \psi & E_0^{-+} \end{pmatrix},$$

where the function  $\rho_h \in \mathcal{C}_0^\infty(U_{2h})$  satisfies

$$\|(h\partial_x)^\alpha \rho_h\|_{L^\infty((a, b))} \leq C_\alpha, \quad \alpha \in \mathbb{N} \quad \text{and} \quad \rho_h \equiv 1 \text{ on } U_{\frac{5h}{4}},$$

after recalling  $U_t = \{x \in (a, b), d(x, U) \leq t\}$ . In particular this implies  $W^h(1 - \rho_h) = 0$ . A direct calculation gives

$$\mathcal{H}_\zeta(z) \mathcal{F}_\zeta(z) = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

$$\begin{aligned} \text{with} \quad A &= 1 + [(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1}(1 - \psi) - [(h\partial_x)^2, \chi_h] E_0 \psi, \\ B &= (H_\zeta^h - z) \chi_h E_0^+ + \chi_h R_0^- E_0^{-+}, \\ C &= R_0^+ (\chi_h E_0 \psi + (1 - \rho_h)(\tilde{H}_\zeta^h - z)^{-1}(1 - \psi)), \\ D &= R_0^+ \chi_h E_0^+, \end{aligned}$$

where we have used  $H_\zeta^h \chi_h = H_D^h \chi_h = P^h \chi_h$ .

**Proposition 5.3.** Assume the conditions (5.4)(5.5)(5.6) and suppose  $z, \zeta \in \omega_{ch}$ . The matricial operator  $\mathcal{F}_\zeta(z)$  is an approximate inverse of  $\mathcal{H}_\zeta(z)$ :

$$\mathcal{H}_\zeta(z)\mathcal{F}_\zeta(z) = 1 + \mathcal{K}_\zeta(z) \quad \text{and} \quad \mathcal{F}_\zeta(z)\mathcal{H}_\zeta(z) = 1 + \mathcal{K}'_\zeta(z), \quad (5.9)$$

for  $h > 0$  small enough and after adjusting the parameter  $\eta > 0$  so that  $\|\mathcal{K}_\zeta(z)\| + \|\mathcal{K}'_\zeta(z)\| < 1$  according to:

$$\|\mathcal{K}_\zeta(z)\| + \|\mathcal{K}'_\zeta(z)\| \leq C_{a,b,c} e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}. \quad (5.10)$$

More precisely the remainder term equals

$$\mathcal{K}_\zeta(z) = \begin{pmatrix} [(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1}(1 - \psi) - [(h\partial_x)^2, \chi_h] E_0 \psi & -[(h\partial_x)^2, \chi_h] E_0^+ \\ R_0^+(\chi_h - 1)E_0 \psi + R_0^+(1 - \rho_h)(\tilde{H}_\zeta^h - z)^{-1}(1 - \psi) & R_0^+(\chi_h - 1)E_0^+ \end{pmatrix}$$

and is estimated by

$$\mathcal{K}_\zeta(z) = \begin{pmatrix} \mathcal{O}(e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}) & \mathcal{O}(\frac{e^{-\frac{S_0}{h}}}{h}) \\ \mathcal{O}(e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}) & \mathcal{O}(\frac{e^{-\frac{S_0}{h}}}{h^2}) \end{pmatrix}.$$

**Proof:** Set  $\mathcal{K}_\zeta(z) = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}$  and remember the expressions of  $A, B, C, D$  in  $\mathcal{H}_\zeta(z)\mathcal{F}_\zeta(z) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ .

The first coefficient  $K_{11}$  is simply  $A - 1$  according to the above definition.

The coefficient  $K_{12} = B$  is computed by making use of  $H_\zeta^h \chi_h = H_D^h \chi_h$  and of the relation  $(H_D^h - z)E_0^+ + R_0^- E_0^{-+} = 0$  coming from  $\mathcal{H}_D(z)\mathcal{E}_D(z) = 1$ .

The coefficient  $K_{21} = C$  is computed after using the relation  $R_0^+ E_0 = 0$  coming from  $\mathcal{H}_D(z)\mathcal{E}_D(z) = 1$ .

The coefficient  $K_{22} = D - 1$  is computed after using  $R_0^+ E_0^+ = 1$ .

**Estimate of  $K_{11}$ :** For the first term, remark the identity:

$$[(h\partial_x)^2, \rho_h] = 2(h\rho'_h)(h\partial_x) + (h^2\rho''_h), \quad (5.11)$$

where the coefficients  $h\rho'_h$  and  $h^2\rho''_h$  are uniformly bounded and supported in  $U_{2h}$ . Then, owing to Proposition 4.7, it is estimated with:

$$\|[(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1}(1 - \psi)\| \leq C_{a,b,c} e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}. \quad (5.12)$$

For the second term, we have the identity (5.11), where  $\rho_h$  is replaced by  $\chi_h$  and the coefficients  $h\chi'_h$  and  $h^2\chi''_h$  are uniformly bounded and supported in  $\{x \in (a, b), d(x, \{a, b\}) < h\}$ .

By introducing a circle  $\gamma_0 = \{z' \in \mathbb{C}, |z' - \lambda^0| = \frac{2}{c}h\}$ , the formula

$$E_0(z) = (H_D^h - z)^{-1}(1 - \Pi^h) = -\frac{1}{2i\pi} \int_{\gamma_0} \frac{1}{z' - z} \frac{1}{(z' - H_D^h)} dz',$$

and Proposition 4.1-ii) imply

$$\|[(h\partial_x)^2, \chi_h] E_0 \psi\| \leq \frac{C_{a,b,c} e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}}{h^3}. \quad (5.13)$$

**Estimate of  $K_{21}$ :** The cut-off  $(\chi_h - 1)$  is supported in  $\{x \in (a, b), d(x, \{a, b\}) < h\}$ . Meanwhile we verify with the same argument as for (5.13) that the function  $u = E_0 \psi f$  satisfies

$$\|e^{\frac{x}{h}} u\| \leq \frac{C_{a,b,c} \|f\|}{h^3},$$



for  $\varphi = d_{Ag}(x, \text{supp } \psi, V, \lambda^0)$ . The operator  $R_0^+$  is the finite rank operator defined by taking the scalar product with  $\Phi_j^h$ ,  $j = 1, \dots, \ell$ . With the exponential decay of the eigenfunctions  $\Phi_j^h$ ,  $j = 1, \dots, \ell$ , stated in Proposition 4.1, we get:

$$\|R_0^+(1 - \chi_h)E_0\psi\| \leq C_{a,b,c}e^{-\frac{3S_0 - C_{a,b,c}\eta}{2h}}.$$

The second term is estimated like the first one of  $K_{11}$  while replacing  $[(h\partial_x)^2, \rho_h]$  with  $R_0^+(1 - \rho_h)$ :

$$\|R_0^+(1 - \rho_h)(\tilde{H}_\zeta^h - z)^{-1}(1 - \psi)\| \leq C_{a,b,c}e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}}.$$

**Estimate of  $K_{12}$  and  $K_{22}$ :** The operator  $E_0^+$  is defined by  $E_0^+v^+ = \sum_{j=1}^\ell v_j \Phi_j^h$  and the exponential decay of the eigenfunctions  $\Phi_j^h$ ,  $j = 1, \dots, \ell$ , stated in Proposition 4.1 with the relation (5.11), where  $\rho_h$  is replaced by  $\chi_h$ , yields

$$\|K_{12}\| = \|[(h\partial_x)^2, \chi_h]E_0^+\| \leq C_{a,b,c}\frac{e^{-\frac{S_0}{h}}}{h}. \quad (5.14)$$

For  $K_{22}$  we use additionally the exponential decay of the  $\Phi_j^h$ ,  $j = 1, \dots, \ell$  contained in  $R_0^+$  and we get

$$\|K_{22}\| = \|R_0^+(1 - \chi_h)E_0^+\| \leq C_{a,b,c}\frac{e^{-\frac{2S_0}{h}}}{h^2}. \quad (5.15)$$

**Left and Right inverse:** When  $h$  and  $\eta$  are small enough the previous analysis says that  $\mathcal{F}_\zeta(z)(1 + \mathcal{K}_\zeta(z))^{-1}$  is a right-inverse of  $\mathcal{H}_\zeta(z)$  and  $\mathcal{H}_\zeta(z)$  is surjective.

From the definitions (4.8) and (4.9), we have:

$$\tilde{H}_\zeta^h = \tilde{H}^h\left(\zeta^{\frac{1}{2}}\right) \quad \text{and} \quad H_\zeta^h = H^h\left(\zeta^{\frac{1}{2}}\right). \quad (5.16)$$

After two integrations by part, we get  $\left(H^h\left(\zeta^{\frac{1}{2}}\right)\right)^* = H^h\left(-(\bar{\zeta})^{\frac{1}{2}}\right)$ . With  $(R_0^+)^* = R_0^-$  and with the notations induced by (5.8) and (5.16), we obtain  $\left[\mathcal{H}(\zeta^{\frac{1}{2}}, z)\right]^* = \mathcal{H}(-(\bar{\zeta})^{\frac{1}{2}}, \bar{z})$ . The analysis performed to obtain (5.10) for  $\mathcal{K}(\zeta^{\frac{1}{2}}, z)$  can be adapted in the case of  $\mathcal{K}(-(\bar{\zeta})^{\frac{1}{2}}, \bar{z})$ : this yields the surjectivity of  $\mathcal{H}(-(\bar{\zeta})^{\frac{1}{2}}, \bar{z})$ . Since

$$\text{Ker}\left(\mathcal{H}(\zeta^{\frac{1}{2}}, z)\right) = \left[\text{Ran}\left(\mathcal{H}(\zeta^{\frac{1}{2}}, z)\right)^*\right]^\perp = \{0\},$$

the injectivity of  $\mathcal{H}(\zeta^{\frac{1}{2}}, z)$  follows. □

**Notation:** When  $h > 0$  is small enough, we set

$$\mathcal{E}_\zeta(z) = \begin{pmatrix} E & E^+ \\ E^- & E^{-+} \end{pmatrix} = \mathcal{H}_\zeta(z)^{-1}. \quad (5.17)$$

The Schur complement formula

$$(H_\zeta^h - z)^{-1} = E - E^+(E^{-+})^{-1}E^- \quad (5.18)$$

recalls that  $(H_\zeta^h - z)$  is invertible if and only if the  $\ell \times \ell$  square matrix  $E^{-+}$  is invertible. An accurate calculation of this matrix allows to identify the poles of  $(H_\zeta^h - z)^{-1}$ .

The final result comes from a higher order estimate after taking the Neumann series

$$(1 + \mathcal{K}_\zeta(z))^{-1} = 1 - \mathcal{K}_\zeta(z) + \mathcal{K}_\zeta(z)^2 - \mathcal{K}_\zeta(z)^3 + \mathcal{K}_\zeta(z)^4 + \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}).$$

**Proposition 5.4.** *Assume the conditions (5.4)(5.5)(5.6) and suppose  $z, \zeta \in \omega_{ch}$ . Then*

$$E^{-+} = E_0^{-+} + \mathcal{O}(e^{-\frac{2S_0}{h}}h^{-3}),$$

and

$$E^{-+} = E_0^{-+} - E_0^- [(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+ - E_0^{-+} R_0^+ (\chi_h - 1) E_0^+ \\ - E_0^{-+} R_0^+ (1 - \rho_h) (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+ + \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}).$$

**Proof:** We compute first the coefficients  $K_{12}^{(2)}$  and  $K_{22}^{(2)}$  where  $\mathcal{K}_\zeta(z)^n = \begin{pmatrix} K_{11}^{(n)} & K_{12}^{(n)} \\ K_{21}^{(n)} & K_{22}^{(n)} \end{pmatrix}$ .

$\mathbf{K}_{12}^{(2)} = \mathbf{K}_{11}\mathbf{K}_{12} + \mathbf{K}_{12}\mathbf{K}_{22}$ : Due to the support condition when  $\eta > 0$  is chosen small enough and  $h > 0$  is small enough, the first term equals:

$$K_{11}K_{12} = -[(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+,$$

and with the same argument as for (5.12) we get:

$$\|K_{11}K_{12}\| \leq \frac{C_{a,b,c}}{h^2} e^{-\frac{2S_0}{h}}, \quad (5.19)$$

where some additional exponential decay comes from the eigenfunctions appearing in  $E_0^+$  and the support of the derivatives of  $\chi_h$ . From the equations (5.14) and (5.15), the second term satisfies

$$\|K_{12}K_{22}\| \leq \|K_{12}\| \|K_{22}\| \leq \frac{C_{a,b,c}}{h^3} e^{-\frac{3S_0}{h}}.$$

$\mathbf{K}_{22}^{(2)} = \mathbf{K}_{21}\mathbf{K}_{12} + \mathbf{K}_{22}^2$ : The first term equals

$$K_{21}K_{12} = -R_0^+ (1 - \rho_h) (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+,$$

and as it was done for (5.19), we obtain:

$$\|K_{21}K_{12}\| \leq \frac{C_{a,b,c}}{h^3} e^{-\frac{2S_0}{h}}.$$

Then, from equation (5.15), the second term verifies

$$\|K_{22}^2\| \leq \|K_{22}\|^2 \leq \frac{C_{a,b,c}}{h^4} e^{-\frac{4S_0}{h}}.$$

**Estimate of  $K_{12}^{(3)}$ ,  $K_{22}^{(3)}$ ,  $K_{12}^{(4)}$  and  $K_{22}^{(4)}$ :** A direct computation gives for  $i = 1$  and  $2$ :

$$K_{i2}^{(n+1)} = K_{i1}K_{12}^{(n)} + K_{i2}K_{22}^{(n)},$$

and (5.10) implies:

$$\|K_{i2}^{(n+1)}\| \leq \|\mathcal{K}_\zeta(z)\| (\|K_{12}^{(n)}\| + \|K_{22}^{(n)}\|) \leq C_{a,b,c} e^{-\frac{S_0 - C_{a,b,c}\eta}{2h}} (\|K_{12}^{(n)}\| + \|K_{22}^{(n)}\|).$$

Moreover, we have obtained:

$$K_{12}^{(2)} = \mathcal{O}(e^{-\frac{2S_0 - C_{a,b,c}\eta}{h}}) \quad \text{and} \quad K_{22}^{(2)} = \mathcal{O}(e^{-\frac{2S_0 - C_{a,b,c}\eta}{h}}),$$

therefore we have:

$$K_{12}^{(3)} = \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}), \quad K_{22}^{(3)} = \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}), \\ K_{12}^{(4)} = \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}), \quad K_{22}^{(4)} = \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}).$$

**Computing  $E^{-+}$ :** We have

$$E^{-+} - E_0^{-+} = E_0^- \psi [-K_{12} + K_{12}^{(2)} - K_{12}^{(3)} + K_{12}^{(4)}] + E_0^{-+} [-K_{22} + K_{22}^{(2)} - K_{22}^{(3)} + K_{22}^{(4)}] + \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}).$$

Since the operators  $E_0^- \psi$  and  $E_0^{-+}$  are uniformly bounded, it follows from  $E_0^- \psi K_{12} = 0$  and  $K_{22} = \mathcal{O}(e^{-\frac{2S_0}{h}} h^{-2})$  that:

$$E^{-+} - E_0^{-+} = \mathcal{O}(e^{-\frac{2S_0}{h}} h^{-3})$$

and

$$\begin{aligned} E^{-+} - E_0^{-+} &= E_0^- \psi K_{11} K_{12} - E_0^{-+} K_{22} + E_0^{-+} K_{21} K_{12} + \mathcal{O}(e^{-\frac{5S_0 - c_{abc}\eta}{2h}}) \\ &= -E_0^- [(h\partial_x)^2, \rho_h] (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+ - E_0^{-+} R_0^+ (\chi_h - 1) E_0^+ \\ &\quad - E_0^{-+} R_0^+ (1 - \rho_h) (\tilde{H}_\zeta^h - z)^{-1} [(h\partial_x)^2, \chi_h] E_0^+ + \mathcal{O}(e^{-\frac{5S_0 - C_{abc}\eta}{2h}}). \end{aligned}$$

□

### 5.3 Localization of the resonances

In what follows we discuss the problem of resonances for the operator  $H_{\theta_0, V-W^h}^h(0)$ . Using (5.18) and the detecting method introduced in Subsection 5.1, these coincides with the singularities of the matrix  $(E^{-+}(z, ze^{-2\theta_0} z))^{-1}$  in a sector  $\arg(z) \in (-2\tau, 0)$  for a suitable  $\tau$ . Here the symbol  $E^{-+}(z, \zeta)$  actually denotes the  $(z, \zeta)$ -dependent matrix defined in (5.17). The comparison of the Schur complements  $E^{-+}$  and  $E_0^{-+}$  stated in Proposition 5.4, allows to state the following localization result on the resonances of the operator  $H_{V-W^h, \theta_0}^h(0)$  and to estimate accurately their variations w.r.t  $\theta_0$ .

**Proposition 5.5.** *Assume the conditions (5.4)(5.5)(5.6) and fix  $\theta_0$  such that  $|\theta_0| \leq \frac{c^2 h}{8}$ . Then for  $h > 0$  small enough, the operator  $H_{\theta_0, V-W^h}^h(0)$  has exactly  $\ell$  resonances  $\{z_1^h(\theta_0), \dots, z_\ell^h(\theta_0)\}$  in  $\omega_{\frac{ch}{2}}$ , possibly counted with multiplicities, with the estimate*

$$z_j^h(\theta_0) - \lambda_j^h = \mathcal{O}\left(\frac{e^{-\frac{2S_0}{h}}}{h^3}\right),$$

after the proper labelling with respect to  $j \in \{1, \dots, \ell\}$ .

In particular, when

$$\lim_{h \rightarrow 0} h^3 e^{\frac{2S_0}{h}} \min_{j \neq j'} |\lambda_j^h - \lambda_{j'}^h| = +\infty, \quad (5.20)$$

there exists  $T_{a,b,c} > 1$ , such that every disc  $D_{j,h}(T) = \left\{z \in \mathbb{C}, |z - \lambda_j^h| \leq T \frac{e^{-\frac{2S_0}{h}}}{h^3}\right\}$  contains exactly one resonance  $z_j(\theta_0)$  when  $T$  is fixed so that  $T \geq T_{a,b,c}$  and  $h > 0$  is small enough.

**Proof:** We look for the points where the matrix  $E^{-+}(z, ze^{-2\theta_0})$  is not invertible. When  $z \in \omega_{\frac{ch}{2}}$ , then  $|z| \leq \frac{2}{c}$  when  $h$  is small enough and the two points  $z$  and  $\zeta = ze^{-2\theta_0} = z + z(e^{2\theta_0} - 1)$  belong to  $\omega_{ch}$ . Thus, Proposition 5.4 gives

$$\|E^{-+}(z, ze^{-2\theta_0}) - E_0^{-+}(z)\|_\infty \leq M_{a,b,c} \frac{e^{-\frac{2S_0}{h}}}{h^3}, \quad (5.21)$$

where the equivalent norm  $\|a_{ij}\|_\infty = \max_{i,j} |a_{ij}|$  is used.

Let  $\Omega_h = \left\{z \in \mathbb{C}; \min_{1 \leq j \leq \ell} |z - \lambda_j^h| < 2\ell M_{a,b,c} \frac{e^{-\frac{2S_0}{h}}}{h^3}\right\}$  and suppose  $z \notin \Omega_h$ . Then the coefficients

$E_{ij}^{-+}$  of  $E^{-+}$  are such that for all  $i \in \{1, \dots, \ell\}$ ,  $|E_{ii}^{-+}| > \sum_{\substack{j=1 \\ j \neq i}}^{\ell} |E_{ij}^{-+}|$  and  $E^{-+}$  is invertible by

Gershgorin circle theorem.

To conclude the proof, we have to compare the number of resonances to the number of Dirichlet

eigenvalues in each connected component  $\Omega_{j,h}$  of  $\Omega_h$  ( $\Omega_{j,h} = \Omega_{j',h}$  is not forbidden). Defining  $E^{-+}(t) = E_0^{-+} + t(E^{-+} - E_0^{-+})$  for  $0 \leq t \leq 1$ , the number  $N(t)$  of points in  $\Omega_{j,h}$  such that  $E^{-+}(t)$  is not invertible, is constant on  $[0, 1]$ . Actually, note first that (5.21) implies that for all  $t \in [0, 1]$ ,  $E^{-+}(t)$  is invertible when  $z \in \partial\Omega_{j,h}$ , using an argument similar to the one used for  $E^{-+}$  outside  $\Omega_h$ . Therefore, for any  $t_0 \in [0, 1]$  the analyticity of  $E^{-+}(t_0)$  with respect to  $z$  implies

$$\inf_{z \in \partial\Omega_{j,h}} |\det E^{-+}(t_0)| > 0,$$

and for  $\delta$  small enough, the estimate:

$$\begin{aligned} |\det E^{-+}(t_0 + \delta) - \det E^{-+}(t_0)| &= |\det(E^{-+}(t_0) + \delta(E^{-+} - E_0^{-+})) - \det E^{-+}(t_0)| = |\delta| |R(t_0, \delta)| \\ &< \inf_{z \in \partial\Omega_{j,h}} |\det E^{-+}(t_0)| \leq |\det E^{-+}(t_0)| \end{aligned}$$

holds for all  $z \in \partial\Omega_{j,h}$  after noticing that the function  $|R(t_0, \delta)|$  is a bounded polynomial of  $t_0$ ,  $\delta$  and of the coefficients of  $E_0^{-+}$  and  $E^{-+}$ . The functions  $\det(E^{-+}(t_0))$  and  $\det E^{-+}(t_0 + \delta)$  are holomorphic functions of  $z \in \omega_{\frac{ch}{2}}$  such that  $\sup_{z \in \partial\Omega_{j,h}} \left| \frac{\det E^{-+}(t_0 + \delta)}{\det E^{-+}(t_0)} - 1 \right| < 1$ . Thus, Rouché's theorem implies  $N(t_0 + \delta) = N(t_0)$ . The function  $N(t)$  is continuous on  $[0, 1]$  with integer values. It is constant.

Assuming  $e^{\frac{2S_0}{h}} h^3 |\lambda_j^h - \lambda_{j'}^h| \rightarrow +\infty$  for all pair of distinct  $j, j'$ , implies  $\Omega_{j,h} \subset D_{j,h}(R)$  for all the  $j$ 's with  $D_{j,h}(R) \cap D_{j',h}(R) = \emptyset$  if  $j \neq j'$  when  $R \geq 2\ell M_{a,b,c}$  and  $h$  is small enough. This yields the last statement.  $\square$

**Remark 5.6.** In the above proposition the term resonances is used for the eigenvalues of the operator  $H_{ze^{-2\theta_0}}^h$ , which in principle may still have a positive imaginary part. In the particular case of  $\theta_0 = i\tau$ ,  $\tau \in (0, \frac{\pi}{4})$ , the result of Lemma 5.1 implies that these eigenvalues must lay in the lower half complex plane. On the other hand, the result of next proposition and the lower bound on  $|\operatorname{Im} z_j^h(0)|$  (see Proposition 5.8) implicitly yields:  $\operatorname{Im} z_j^h(\theta_0) < 0$  on a suitable range of  $|\theta_0|$ . Under each of such conditions the points  $z_j^h(\theta_0)$  corresponds to resonances of the operator  $H_{\theta_0, V-W^h}^h(0)$  as defined in Proposition 3.6.

The next Proposition localizes the resonances  $z_j^h(\theta_0)$  of  $H_{\theta_0, V-W^h}^h(0)$  with respect to the resonances  $z_j^h := z_j^h(0)$  of  $H_{0, V-W^h}^h(0)$  by making use of the comparison between  $E^{-+}(z, ze^{-2\theta_0})$  and  $E^{-+}(z, z)$ .

**Proposition 5.7.** Assume the conditions (5.4)(5.5)(5.6) and  $e^{-\frac{S_0}{4h}} \leq |\theta_0| \leq \frac{c^2 h}{8}$ . Then for  $h > 0$  small enough, the matrices  $E^{-+}$  of Proposition 5.4 associated with  $\zeta = z$  and  $\zeta = ze^{-2\theta}$  satisfy

$$\sup_{z \in \omega_{\frac{ch}{2}}} |E^{-+}(z, ze^{-2\theta_0}) - E^{-+}(z, z)| = \mathcal{O} \left( |\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^3} \right). \quad (5.22)$$

If additionally (5.20) is assumed the variation of the resonances around  $\lambda^0$  for  $e^{-\frac{S_0}{4h}} \leq |\theta_0| \leq \frac{c^2 h}{8}$  and  $\theta_0 = 0$  is estimated by

$$\max_{j \in \{1, \dots, \ell\}} |z_j^h(\theta_0) - z_j^h| = \mathcal{O} \left( |\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^3} \right).$$

**Proof:** For  $z \in \omega_{\frac{ch}{2}}$  and  $\theta_0$  such that  $|\theta_0| \leq \frac{c^2 h}{8}$ , the Proposition 5.4 implies that:

$$\begin{aligned} E^{-+}(z, ze^{-2\theta_0}) - E^{-+}(z, z) &= E_0^{-} [(h\partial_x)^2, \rho_h] D[(h\partial_x)^2, \chi_h] E_0^{+} \\ &\quad + E_0^{-+} R_0^{+} (1 - \rho_h) D[(h\partial_x)^2, \chi_h] E_0^{+} + \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}) \\ &= I + II + \mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}}), \end{aligned}$$

where  $D = (\tilde{H}_z^h - z)^{-1} - (\tilde{H}_{ze^{-2\theta_0}}^h - z)^{-1}$ . The operator  $E_0^-$  being bounded, the first term  $I$  is estimated as we did for (5.19) where  $(\tilde{H}_\zeta^h - z)^{-1}$  is replaced by  $D$  and we use Proposition 4.8 instead of Proposition 4.7. This leads to:

$$||I|| \leq C_{a,b,c} |z^{1/2} - (ze^{-2\theta_0})^{1/2}| \frac{e^{-\frac{2S_0}{h}}}{h^3} \leq C_{a,b,c} |\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^3}.$$

For  $II$ , using the exponential decay given by the operator  $R_0^+$ , we get:

$$||II|| \leq C_{a,b,c} |\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^3}.$$

The assumption  $e^{-\frac{S_0}{4h}} \leq |\theta_0|$  ensures that the remainder  $\mathcal{O}(e^{-\frac{5S_0 - C_{a,b,c}\eta}{2h}})$  is absorbed by  $|\theta_0| e^{-\frac{2S_0}{h}} h^{-3}$  as  $h \rightarrow 0$ . We have proved (5.22).

When (5.20) is verified, Proposition 5.5 says that every disc  $D_{j,h}(T) = \{z \in \mathbb{C}, |z - \lambda_j^h| < Te^{-\frac{2S_0}{h}} h^{-3}\}$  for any  $T \geq T_{a,b,c}$ , contains exactly one resonance  $z_j^h(\theta_0)$ , and in particular one resonance  $z_j^h$  when  $\theta_0 = 0$ . Hence the matrix  $E^{-+}(z, z)$  has only simple poles and its inverse is the meromorphic function

$$(E^{-+}(z, z))^{-1} = \sum_{j=1}^{\ell} \frac{A_j^h}{z - z_j^h} + F^h(z), \quad z \in \omega_{\frac{e^h}{2}}. \quad (5.23)$$

The matrix  $A_j^h$  is nothing but the residue

$$A_j^h = \frac{1}{2i\pi} \int_{\partial D_{j,h}(T)} (E^{-+}(z, z))^{-1} dz,$$

while the function  $F^h(z)$  is a holomorphic function estimated via the maximum principle by

$$\sup_{z \in \omega_{\frac{e^h}{4}}} |F^h(z)| \leq \sup_{z \in \partial \omega_{\frac{e^h}{4}}} \left[ |(E^{-+}(z, z))^{-1}| + \sum_{j=1}^{\ell} \frac{|A_j^h|}{|z - z_j^h|} \right]. \quad (5.24)$$

The estimate of Proposition 5.4 says

$$|E^{-+}(z, z) - E_0^{-+}(z)| \leq C_{a,b,c} \frac{e^{-\frac{2S_0}{h}}}{h^3},$$

while we know  $|(E_0^{-+}(z))^{-1}| \leq \max_{1 \leq j \leq \ell} |z - \lambda_j^h|^{-1}$ . After writing

$$(E^{-+})^{-1} = [1 + (E_0^{-+})^{-1}(E^{-+} - E_0^{-+})]^{-1} (E_0^{-+})^{-1}, \quad (5.25)$$

we get for  $T > \max\{T_{a,b,c}, 2C_{a,b,c}\}$

$$\sup_{z \in \partial D_{j,h}(T)} |(E^{-+}(z, z))^{-1}| \leq \frac{h^3 e^{\frac{2S_0}{h}}}{T[1 - \frac{C_{a,b,c}}{T}]} \leq \frac{2h^3 e^{\frac{2S_0}{h}}}{T},$$

and finally the uniform bound for the residues

$$\max_{1 \leq j \leq \ell} |A_j^h| \leq 2.$$

The holomorphic part  $F^h(z)$  is then estimated with (5.24). Actually, the first term is estimated with the help of (5.25) while the second term is treated with the above estimate of  $A_j^h$  and by making use of  $\max_{1 \leq j \leq \ell} |z_j^h - \lambda_j^h| \leq T_{a,b,c} \frac{e^{-\frac{2S_0}{h}}}{h^3}$ :

$$\sup_{z \in \omega_{\frac{e^h}{4}}} |F^h(z)| \leq \frac{C'_{a,b,c}}{h}.$$

For all  $z \in \omega_{\frac{ch}{4}} \setminus \{z_1^h, \dots, z_\ell^h\}$ , the inverse of  $E^{-+}(z, z)$  is thus estimated by

$$|(E^{-+}(z, z))^{-1}| \leq \sum_{j=1}^{\ell} \frac{2}{|z - z_j^h|} + \frac{C'_{a,b,c}}{h}.$$

We now write for  $z \notin \omega_{\frac{ch}{4}} \setminus \{z_1^h, \dots, z_\ell^h\}$

$$E^{-+}(z, ze^{-2\theta_0}) = E^{-+}(z, z) [1 + (E^{-+}(z, z))^{-1}(E^{-+}(z, ze^{-2\theta_0}) - E^{-+}(z, z))] .$$

Due to the estimate (5.22) the condition

$$\min_{j \in \{1, \dots, \ell\}} |z - z_j^h| \geq T \frac{e^{-\frac{2S_0}{h}} |\theta_0|}{h^3}$$

implies

$$|(E^{-+}(z, z))^{-1}(E^{-+}(z, ze^{-2\theta_0}) - E^{-+}(z, z))| \leq \left[ 2\ell \frac{h^3 e^{\frac{2S_0}{h}}}{T|\theta_0|} + C'_{a,b,c} h^{-1} \right] C''_{a,b,c} \frac{|\theta_0| e^{-\frac{2S_0}{h}}}{h^3},$$

where the right-hand side is smaller than 1 if  $T \geq 4\ell C''_{a,b,c}$  and  $h > 0$  is small enough. Outside  $\cup_{j=1}^{\ell} \left\{ z \in \mathbb{C}, |z - z_j^h| \leq T|\theta_0| e^{-\frac{2S_0}{h}} h^{-3} \right\}$ ,  $E^{-+}(z, ze^{-2\theta_0})$  is invertible. For such a  $T$  we have proved

$$\max_{j \in \{1, \dots, \ell\}} |z_j^h(\theta_0) - z_j^h| \leq T \frac{e^{-\frac{2S_0}{h}} |\theta_0|}{h^3}.$$

□

## 5.4 A Fermi-Golden rule

In [21], a Fermi Golden rule for the imaginary parts of resonances  $\Gamma_j = -\text{Im } z_j^h$  in the case  $\theta_0 = 0$  has been introduced. It plays a major role in the analysis of the nonlinear effects studied in [19][20][21][45][46][18] for it expresses accurately how the tunnel effect between the resonant state and the incoming waves is balanced between the left and right-hand sides. By assuming

$$\lim_{h \rightarrow 0} e^{\frac{S_U}{h}} \min_{1 \leq j < j' \leq \ell} |\lambda_j^h - \lambda_{j'}^h| = +\infty \quad \text{with} \quad S_U < \frac{S_0}{8}, \quad (5.26)$$

which is stronger than (5.20), the energy range of  $\lambda \in \mathbb{R}$  associated with the resonance  $z_j^h$  is given by  $|\lambda - z_j^h| \leq e^{-\frac{S_U}{h}}$ . When  $\tilde{\psi}_{-,0}^h(\pm\sqrt{\lambda}, \cdot)$  denote the generalized eigenfunctions of the filled well Hamiltonian  $H_{0,V}^h(0)$  at energy  $\lambda$  defined in section 4.2 and  $\Phi_j^h$ ,  $j \in \{1, \dots, \ell\}$ , denote the normalized eigenfunctions of the Dirichlet Hamiltonian  $H_D^h$  given in (4.3), the formula

$$\Gamma_j^h + o(\Gamma_j^h) = \frac{|\langle W^h \tilde{\psi}_{-,0}^h(\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2 + |\langle W^h \tilde{\psi}_{-,0}^h(-\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2}{4h\sqrt{\lambda}} \geq \frac{e^{-\frac{2S_0}{h}}}{C}, \quad (5.27)$$

for all  $\lambda \in \mathbb{R}$  such that  $|\lambda - z_j^h| \leq e^{-\frac{S_U}{h}}$ , has been proved under additional assumptions about the localization of the  $\Phi_j^h$  within  $\text{supp } W^h$ . We refer to Proposition 7.9 in [21] and to the subsequent explicit computations in Sections 7 and Section 8 of [21] for the details and in particular for the lower bound.

We shall assume that the formula (5.27) is true when  $\theta_0 = 0$  and check that it remains true when  $\theta_0 \neq 0$  is small enough. We shall use the notation

$$\Gamma_j^h = -\text{Im } z_j^h \quad \text{and} \quad \Gamma_j^h(\theta_0) = -\text{Im } z_j^h(\theta_0).$$

**Proposition 5.8.** Assume the conditions (5.4)(5.5)(5.6)(5.26)(5.27) and take  $\theta_0$  such that  $e^{-\frac{S_0}{4h}} \leq |\theta_0| \leq \frac{c^2 h}{8}$  then the Fermi Golden Rule

$$\Gamma_j^h(\theta_0) = \frac{|\langle W^h \tilde{\psi}_{-, \theta_0}^h(\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2 + |\langle W^h \tilde{\psi}_{-, \theta_0}^h(-\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2}{4h\sqrt{\lambda}} + o(\Gamma_j^h) + \mathcal{O}\left(|\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^5}\right) \quad (5.28)$$

holds for all  $\lambda \in \mathbb{R}$  such that  $|\lambda - z_j^h| \leq e^{-\frac{S_\mu}{h}}$ .  
In particular, when  $\lim_{h \rightarrow 0} h^{-5}\theta_0 = 0$  we have

$$\Gamma_j^h(\theta_0) + o(\Gamma_j^h(\theta_0)) = \frac{|\langle W^h \tilde{\psi}_{-, \theta_0}^h(\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2 + |\langle W^h \tilde{\psi}_{-, \theta_0}^h(-\sqrt{\lambda}, \cdot), \Phi_j^h \rangle|^2}{4h\sqrt{\lambda}} \geq \frac{e^{-\frac{2S_0}{h}}}{C}. \quad (5.29)$$

**Proof:** Proposition 5.7 gives:

$$|\Gamma_j^h(\theta_0) - \Gamma_j^h| \leq C_{a,b,c} |\theta_0| \frac{e^{-\frac{2S_0}{h}}}{h^3}. \quad (5.30)$$

Let  $f(\theta_0) = \langle W^h \psi_{-, \theta_0}^h(\sqrt{\lambda}, \cdot), \Phi_j^h \rangle$ . The pointwise and  $L^2$  weighted estimates of  $u = \tilde{\psi}_{-, \theta_0}^h(\sqrt{\lambda}, \cdot) - \tilde{\psi}_{-, 0}^h(\sqrt{\lambda}, \cdot)$  stated in Proposition 4.5 with  $\varphi(x) = d_{Ag}(x, a, V, \lambda)$  say

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} u(x)| + \|e^{\frac{\varphi}{h}} u\|_{L^2} \leq \frac{C'_{a,b,c} |\theta_0|}{h^{3/2}},$$

while Proposition 4.4 gives

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi(x)}{h}} \tilde{\psi}_{-, \theta_0}^h(\sqrt{\lambda}, x)| + \|e^{\frac{\varphi}{h}} \tilde{\psi}_{-, \theta_0}^h(\sqrt{\lambda})\|_{L^2} \leq \frac{C'_{a,b,c}}{h^{1/2}},$$

with the same estimate for  $\theta_0 = 0$ . Moreover, the exponential decay of  $\Phi_j^h$  stated in Proposition 4.1 can be written as

$$h^{1/2} \sup_{x \in [a, b]} |e^{\frac{\varphi_j(x)}{h}} \Phi_j^h(x)| + \|e^{\frac{\varphi_j}{h}} \Phi_j^h\|_{L^2} \leq \frac{C'_{a,b,c}}{h},$$

with  $\varphi_j(x) = d_{Ag}(x, U, V, \lambda_j^h)$ . Recalling that

$$\|W_1^h\|_{L^\infty} \leq \frac{1}{c}, \quad \|W_2^h\|_{\mathcal{M}_b} \leq \frac{h}{c}, \quad \text{supp } W^h \subset \{d(x, U) \leq h\},$$

and  $S_0 = d_{Ag}(U, \{a, b\}, V, \lambda^0) \leq d_{Ag}(x, \{a, b\}, V, \lambda) + \mathcal{O}(h)$  when  $x \in U^h$  and  $|\lambda - z_j^h| \leq e^{-\frac{S_\mu}{h}}$ . Hence we get with our assumptions

$$|f(\theta_0) - f(0)| \leq C''_{a,b,c} |\theta_0| \frac{e^{-\frac{S_0}{h}}}{h^{5/2}}$$

and

$$|f(\theta_0)| \leq C''_{a,b,c} \frac{e^{-\frac{S_0}{h}}}{h^{3/2}}.$$

We obtain

$$\left| \frac{|f(\theta_0)|^2}{4h\sqrt{\lambda}} - \frac{|f(0)|^2}{4h\sqrt{\lambda}} \right| = \mathcal{O}\left(\frac{e^{-\frac{2S_0}{h}} |\theta_0|}{h^5}\right). \quad (5.31)$$

□

**Remark 5.9.** In [21], the Fermi Golden Rule (5.27) has been studied with  $W^h \in L^\infty((a, b))$ . Nevertheless it can be proved in cases when the singular part  $W_2^h$  does not vanish by a direct analysis like for example when  $W_2^h = h\delta_c$ . The presentation of Proposition 5.8 shows that the stability result w.r.t to  $\theta_0$  holds in this more general framework and leaves the possibility of further applications.

## 6 Accurate resolvent estimates for the whole space problem

In the previous sections 4 and 5, we got accurate resolvent estimates with respect to  $h > 0$  for the problem reduced to the interval  $(a, b)$ . We use here this information in order to derive accurate resolvent estimates for  $(H_{\theta_0, V-W^h}(\theta_0) - z)^{-1}$  when  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ , which are essential in the justification of the adiabatic evolution.

### 6.1 Localization of the spectrum

The results of Corollary 3.4, Proposition 3.6, Proposition 5.5 and section 5.1 can be summarized with the corresponding assumptions.

**Proposition 6.1.** *Assume that  $V \in L^\infty((a, b); \mathbb{R})$  and  $W^h = W_1^h + W_2^h \in \mathcal{M}_b((a, b))$  are real valued with the hypothesis (4.1),*

$$c1_{(a,b)} \leq V \quad , \quad \|V\|_{L^\infty} \leq \frac{1}{c} \quad , \quad \|W_1^h\| \leq \frac{1}{c} \quad , \quad \|W_2^h\| \leq \frac{h}{c} \quad ,$$

$W_1^h$  and  $W_2^h$  are supported in the domain  $U_h = \{x \in (a, b); d(x, U) \leq h\}$  where  $U$  is a fixed compact subset of  $(a, b)$ . Assume also  $\theta_0 = ih^{N_0}$  with  $N_0 > 1$  and  $h < h_0$ . Then:

a)  $\sigma_{ess}(H_{\theta_0, V-W^h}^h(\theta_0)) = \sigma_{ess}(H_{ND, V-W^h}^h(\theta_0)) = e^{-2\theta_0} \mathbb{R}_+$ ;

b) The equality (3.34) written with  $\theta = \theta_0$

$$\begin{aligned} \left(H_{\theta_0, V-W^h}^h(\theta_0) - z\right)^{-1} &= \left(H_{ND, V-W^h}^h(\theta_0) - z\right)^{-1} \\ &\quad - \sum_{i,j,k=1}^4 \left(Bq(z, \theta_0, V - W^h) - A\right)_{ij}^{-1} B_{jk} \langle \gamma(\underline{e}_k, \bar{z}, \bar{\theta}_0), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta_0) \end{aligned} \quad (6.1)$$

holds as an identity of meromorphic functions on  $\mathbb{C} \setminus e^{-2\theta_0} \mathbb{R}_+$ .

c) In  $\Sigma_h = \{z \in \mathbb{C}, c \leq \operatorname{Re} z \leq \inf_{x \in (a,b)} V(x) - c, |\arg z| < 2|\operatorname{Im} \theta_0|\}$ , the (discrete) spectrum of  $H_{\theta_0, V-W^h}^h(\theta_0)$  is made of eigenvalues  $z^h$  which satisfy  $\operatorname{Ker}(H_{z^h e^{-2\theta_0}}^h - z^h) \neq \{0\}$  where  $H_\zeta^h$  is the operator defined in (4.9). When the spectrum of the Dirichlet Hamiltonian  $\sigma(H_D^h)$  is made of clusters such that (5.4) and (5.6) are satisfied, then there exists  $\kappa_{a,b,c} > 0$  such that

$$\forall z^h \in \Sigma_h \cap \sigma(H_{\theta_0, V-W^h}^h(\theta_0)), \quad d(z^h, \sigma(H_D^h)) \leq e^{-\frac{\kappa_{a,b,c}}{h}}.$$

The resolvent of  $H_{\theta_0, V-W^h}^h(\theta_0)$  will be studied in a domain surrounding a single cluster of eigenvalues  $z^h$ , i.e. with  $\lim_{h \rightarrow 0} z^h = \lambda^0$ , with a distance to  $\sigma(H_{\theta_0, V-W^h}^h(\theta_0))$  bounded from below by  $\frac{1}{C_{a,b,c}} h^{N_0}$ .

**Definition 6.2.** The complex domain  $G_h(\lambda^0)$  is chosen accordingly to the constants  $a, b, c$  involved in the assumptions on  $V$ ,  $W^h$ , the hypotheses (4.1)(5.4)(5.5)(5.6) and to  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ :

$$G_h(\lambda^0) := \left\{ z \in \mathbb{C}, |\operatorname{Re} z - \lambda^0| \leq \Xi_{a,b,c} h, |\arg z| \leq h^{N_0} \text{ and } d(z, \sigma(H_D^h)) \geq \frac{h^{N_0}}{\Xi_{a,b,c}} \right\}, \quad (6.2)$$

for some constant  $\Xi_{a,b,c} > 0$  chosen large enough.



## 6.2 Estimates of the finite rank part

We study here the finite rank part of (6.1):

$$\Upsilon^h(z, V - W^h) = \sum_{i,j,k=1}^4 (Bq(z, \theta_0, V - W^h) - A)_{ij}^{-1} B_{jk} \langle \gamma(\underline{e}_k, \bar{z}, \bar{\theta}_0), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta_0), \quad (6.3)$$

and its variations between the case  $W^h = 0$  and  $W^h \neq 0$ . Every factor will be considered separately. Hence it is convenient to keep the notation  $\gamma_{V-W^h}(\underline{e}_i, z, \theta)$  for the total potential  $V - W^h$  and  $\gamma_V(\underline{e}_i, z, \theta)$  when  $W^h \equiv 0$ .

**Proposition 6.3.** *Assume the hypotheses (4.1) (5.4)(5.5)(5.6). Take  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ , and let  $G_h(\lambda^0)$  be the set defined by (6.2). The matrices  $(Bq(z, \theta_0, V - W^h) - A)^{-1}$  and  $(Bq(z, \theta_0, V) - A)^{-1}$  verify the uniform estimate*

$$\forall z \in G_h(\lambda^0), \quad |(Bq(z, \theta_0, V - W^h) - A)^{-1}| + |(Bq(z, \theta_0, V) - A)^{-1}| \leq C_{a,b,c}h, \quad (6.4)$$

in any fixed matricial norm.

The functions  $\gamma_V$  satisfy the uniform estimates

$$\text{supp } \gamma_V(\underline{e}_{2,3}, z, \theta_0) = \text{supp } \gamma_V(\underline{e}_{2,3}, \bar{z}, \bar{\theta}_0) \subset [a, b], \quad (6.5)$$

$$\text{supp } \gamma_V(\underline{e}_1, z, \theta_0) = \text{supp } \gamma_V(\underline{e}_1, \bar{z}, \bar{\theta}_0) \subset [b, +\infty), \quad (6.6)$$

$$\text{supp } \gamma_V(\underline{e}_4, z, \theta_0) = \text{supp } \gamma_V(\underline{e}_4, \bar{z}, \bar{\theta}_0) \subset (-\infty, a], \quad (6.7)$$

$$\max_{i=2,3} \|\gamma_V(\underline{e}_i, z, \theta_0)\|_{H^{1,h}((a,b))} + \|\gamma_V(\underline{e}_i, \bar{z}, \bar{\theta}_0)\|_{H^{1,h}((a,b))} \leq \frac{C_{a,b,c}}{h^{3/2}}, \quad (6.8)$$

$$\max_{i=1,4} \|\gamma_V(\underline{e}_i, z, \theta_0)\|_{H^{1,h}(\mathbb{R} \setminus [a,b])} + \|\gamma_V(\underline{e}_i, \bar{z}, \bar{\theta}_0)\|_{H^{1,h}(\mathbb{R} \setminus [a,b])} \leq \frac{C_{a,b,c}}{h^{(N_0+1)/2}} \quad (6.9)$$

holds when  $z \in G_h(\lambda^0)$  and  $\mathcal{V} = V - W^h$  or  $\mathcal{V} = V$ .

Moreover the differences  $(Bq(z, \theta_0, V - W^h) - A)^{-1} - (Bq(z, \theta_0, V) - A)^{-1}$  and  $\gamma_{V-W^h} - \gamma_V$  are estimated by

$$|(Bq(z, \theta_0, V - W^h) - A)^{-1} - (Bq(z, \theta_0, V) - A)^{-1}| \leq C_{a,b,c}e^{-\frac{S_0}{2h}}, \quad (6.10)$$

$$\max_{i=2,3} \|\gamma_{V-W^h}(\underline{e}_i, z, \theta_0) - \gamma_V(\underline{e}_i, z, \theta_0)\|_{H^{1,h}((a,b))} \leq C_{a,b,c}e^{-\frac{S_0}{2h}}, \quad (6.11)$$

$$\begin{aligned} \text{with } S_0 &= d_{Ag}(\{a, b\}, U, V, \lambda^0), \\ \gamma_{V-W^h}(\underline{e}_i, z, \theta_0) &= \gamma_V(\underline{e}_i, z, \theta_0), \quad \text{for } i = 1, 4, \end{aligned} \quad (6.12)$$

when  $z \in G_h(\lambda^0)$ , with the same result for  $(\bar{z}, \bar{\theta}_0)$ .

The matrix  $Bq(z, \theta_0, \mathcal{V}) - A$  is expressed with boundary values and we will need the next lemma.

**Lemma 6.4.** *Assume (5.5),  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ , and set*

$$\varphi_b(x) = d_{Ag}(x, b, V, \lambda^0), \quad \varphi_a(x) = d_{Ag}(x, a, V, \lambda^0), \quad S_0 = d_{Ag}(\{a, b\}, U, V, \lambda^0).$$

For any  $z \in G_h$ , the solution  $\tilde{u}_2$  (resp  $\tilde{u}_3$ ) to

$$\begin{cases} (\tilde{P}^h - z)\tilde{u}_{2,3} = (-h^2\Delta + V - z)\tilde{u}_{2,3} = 0 \\ \tilde{u}_2(a) = 0, \quad \tilde{u}_2(b) = 1 \quad (\text{resp. } \tilde{u}_3(a) = 1, \quad \tilde{u}_3(b) = 0), \end{cases}$$

verifies:

$$\|\tilde{u}_2\|_{H^{1,h}((a,b))} \leq C_{a,b,c}h^{1/2}, \quad \|e^{\frac{\varphi_b}{h}}\tilde{u}_2\|_{L^2((a,b))} + \|e^{\frac{\varphi_b}{h}}h\tilde{u}_2'\|_{L^2((a,b))} \leq \frac{C_{a,b,c}}{h^{1/2}}, \quad (6.13)$$

$$\text{resp.} \quad \|\tilde{u}_3\|_{H^{1,h}((a,b))} \leq C_{a,b,c}h^{1/2}, \quad \|e^{\frac{\varphi_a}{h}}\tilde{u}_3\|_{L^2((a,b))} + \|e^{\frac{\varphi_a}{h}}h\tilde{u}_3'\|_{L^2((a,b))} \leq \frac{C_{a,b,c}}{h^{1/2}}, \quad (6.14)$$

$$|\tilde{u}_2'(b)| \leq \frac{C_{a,b,c}}{h}, \quad |\text{Im } \tilde{u}_2'(b)| \leq C_{a,b,c}h^{N_0-1}, \quad |\tilde{u}_2'(a)| \leq \frac{C_{a,b,c}}{h^2}e^{-\frac{2S_0}{h}}, \quad (6.15)$$

$$\text{resp.} \quad |\tilde{u}_3'(a)| \leq \frac{C_{a,b,c}}{h}, \quad |\text{Im } \tilde{u}_3'(a)| \leq C_{a,b,c}h^{N_0-1}, \quad |\tilde{u}_3'(b)| \leq \frac{C_{a,b,c}}{h^2}e^{-\frac{2S_0}{h}}. \quad (6.16)$$

For any  $z \in G_h(\lambda^0)$ , the solution  $u_2$  (resp.  $u_3$ ) to (3.24) rewritten as

$$\begin{cases} (P^h - z)u_{2,3} = (-h^2\Delta + V - W^h - z)u_{2,3} = 0 \\ u_2(a) = 0, \quad u_2(b) = 1 \quad (\text{resp. } u_3(a) = 1, \quad u_3(b) = 0), \end{cases}$$

can be compared with  $\tilde{u}_2$  (resp.  $\tilde{u}_3$ ) according to

$$\max_{i \in \{2,3\}} \|u_i - \tilde{u}_i\|_{H^{1,h}} + |u'_i(a) - \tilde{u}'_i(a)| + |u'_i(b) - \tilde{u}'_i(b)| \leq C_{a,b,c} e^{-\frac{3S_0}{4h}}. \quad (6.17)$$

**Proof:** Let us first focus on the case  $W^h = 0$ . It suffices to study the case of  $\tilde{u}_2$ , the result for  $\tilde{u}_3$  being deduced by symmetry.

Consider a real valued function  $u_0 \in C^\infty$  such that  $u_0(b) = 1$ ,  $\text{supp } u_0 \cap [a, b] \subset [b - h, b]$  and:

$$\|(h\partial_x)^\alpha u_0\| \leq C_\alpha, \quad \alpha \in \mathbb{N},$$

and set  $\tilde{u}_2 = u_0 + \tilde{v}$  where  $\tilde{v}$  solves  $(\tilde{H}_D^h - z)\tilde{v} = f$  with  $f = (h\partial_x)^2 u_0 - (V - z)u_0$ . We keep the notation (4.2) for the Dirichlet Hamiltonian associated with  $\tilde{P}^h$ .

Owing to  $V - \text{Re } z \geq c$ , the variational formulation of  $(\tilde{H}_D^h - z)\tilde{u} = f$  with  $\|f\|_{L^2} \leq Ch^{1/2}$  provides  $\|\tilde{v}\|_{H^{1,h}} \leq Ch^{1/2}$  which yields the first estimate of (6.13). With the equation  $-h^2\tilde{v}'' = -(V - z)\tilde{v} + f$  and applying Lemma A.1 to  $\tilde{v}(b - x)$ , we get  $|\tilde{v}'(b)| \leq \frac{Ch^{1/2}}{h^{3/2}}$  and hence the first estimate of (6.15). The second estimate of (6.15) comes similarly from  $|\text{Im } \tilde{v}'(b)| \leq Ch^{N_0-1}$ . It suffices to write that  $w = \tilde{v} - \bar{\tilde{v}}$  solves

$$(\tilde{H}_D^h - z)w = (z - \bar{z})u_0 + (z - \bar{z})\bar{\tilde{v}} = g,$$

where the right-hand side is estimated by  $\|g\|_{L^2} \leq Ch^{1/2}|\text{Im } z| \leq Ch^{N_0+1/2}$ . The estimate for  $|w'(b)|$  follows the same arguments as for  $|\tilde{v}'(b)|$  with  $h^{N_0+1/2}$  instead of  $h^{1/2}$ .

The second estimate of (6.13) is a direct application of Proposition 4.1-i) to  $(\tilde{H}_D^h - z)\tilde{v} = f$  while noticing that  $d_{Ag}(x, b, V, \lambda^0)$  can take the place of  $d_{Ag}(x, \text{supp } f, V, \text{Re } z)$  because  $|\text{Re } z - \lambda^0| = \mathcal{O}(h)$ ,  $\text{supp } f \subset \text{supp } u_0 \subset [b - h, b]$  and  $d_{Ag}(\cdot, \cdot, V, \lambda^0)$  is uniformly Lipschitz on  $[a, b]^2$ . On the interval  $[a, a + h]$  the second derivative of  $\tilde{v}$  satisfies  $-h^2\tilde{v}'' = -(V - z)\tilde{v}$  so that  $\|\tilde{u}_2(a + \cdot)\|_{H^{2,h}((0,h))} \leq \frac{Ce^{-\frac{\varphi_h(a)}{h}}}{h^{1/2}}$  and we apply again Lemma A.1.

The difference  $v = u_2 - \tilde{u}_2$  solves the Dirichlet problem

$$\begin{cases} (P^h - z)v = W^h\tilde{u}_2 \\ v(a) = v(b) = 0, \end{cases}$$

which means  $v = (H_D^h - z)^{-1}(W^h\tilde{u}_2)$ . It suffices to apply Lemma A.2 with  $\|W^h\tilde{u}_2\|_{H^{-1}} \leq C_{a,b}\|W^h\tilde{u}_2\|_{\mathcal{M}_b} \leq C_{a,b,c}e^{-\frac{S_0}{h}}$ . With  $z \in G_h(\lambda^0)$ , this gives  $\|v\|_{H^{1,h}} \leq \frac{C'_{a,b,c}e^{-\frac{S_0}{h}}}{h^{N_0+1}}$ . In  $[a, a + h]$  or in  $[b - h, b]$ , the equation for  $v$  is simply  $h^2v'' = (V - z)v$  and we use again Lemma A.1 to conclude.  $\square$

### Proof of Proposition 6.3:

**a)** First consider the estimate of  $(Bq - A)^{-1}$  in (6.4) and its variation in (6.10). The explicit form of the matrix  $(Bq(z, \theta_0, V - W^h) - A)$ , using the definitions of  $A, B$  and  $q(z, \theta_0, V)$  given respectively in (3.33) and (3.26), can be written

$$(Bq(z, \theta_0, V - W^h) - A) = M(z) + R(z),$$

with

$$M(z) = \frac{1}{h^2} \begin{pmatrix} e^{-\frac{3\theta_0}{2}} & -u'_2(b) \\ \frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} & e^{\frac{\theta_0}{2}} \\ -e^{\frac{\theta_0}{2}} & \frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} \\ u'_3(a) & -e^{-\frac{3\theta_0}{2}} \end{pmatrix}, \quad R(z) = \frac{1}{h^2} \begin{pmatrix} & u'_3(b) & 0 \\ & 0 & 0 \\ 0 & 0 & \\ 0 & -u'_2(a) & \end{pmatrix},$$

where  $u_{2,3}$  has to be replaced by  $\tilde{u}_{2,3}$  when  $W^h \equiv 0$ . According to (6.15)(6.16) and (6.17)

$$\|R(z)\| \leq C_{a,b,c} e^{-\frac{S_0}{2h}}. \quad (6.18)$$

The inverse matrix  $(Bq(z, \theta_0, V - W^h) - A)^{-1}$  is formally given by:

$$(Bq(z, \theta_0, V - W^h) - A)^{-1} = M(z)^{-1} (1 + R(z)M(z)^{-1})^{-1}. \quad (6.19)$$

An explicit computation gives

$$M(z)^{-1} = h^2 \begin{pmatrix} \frac{1}{\Delta^+} \begin{pmatrix} e^{-\frac{\theta_0}{2}} & u'_2(b) \\ -\frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} & e^{-\frac{3\theta_0}{2}} \end{pmatrix} & \\ & \frac{1}{\Delta^-} \begin{pmatrix} -e^{-\frac{3\theta_0}{2}} & -\frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} \\ -u'_3(a) & -e^{-\frac{\theta_0}{2}} \end{pmatrix} \end{pmatrix},$$

with  $\begin{cases} \Delta^+ = e^{-\theta_0} + \frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} u'_2(b), \\ \Delta^- = e^{-\theta_0} - \frac{ih e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} u'_3(a). \end{cases}$

Using  $|\operatorname{Im} u'_2(b)| + |\operatorname{Im} u'_3(a)| \leq C_{a,b,c} h^{N_0-1}$  due to (6.15)(6.16) and (6.17), leads to the lower bounds for  $\Delta^+$  and  $\Delta^-$ . With our choice of the branch cut:  $\frac{e^{\theta_0}}{\sqrt{ze^{2\theta_0}}} = \pm \frac{1}{\sqrt{z}}$ , depending on  $\arg z$ , and one has

$$\begin{aligned} |\Delta^+| &\geq \operatorname{Re} \Delta^+ \geq \cos(\operatorname{Im} \theta_0) - \frac{h}{|z|} |\operatorname{Im} u'_2(b) \operatorname{Re} \sqrt{z} - \operatorname{Re} u'_2(b) \operatorname{Im} \sqrt{z}| \\ &\geq \cos(\operatorname{Im} \theta_0) - C \frac{h}{|z|} \left( h^{N_0-1} \sqrt{|z|} + \frac{1}{h} |\operatorname{Im} \sqrt{z}| \right). \end{aligned}$$

For  $z \in G_h$ , we have  $|\operatorname{Im} \sqrt{z}| \leq Ch^{N_0}$  and one finally gets:  $|\Delta^+| \geq \frac{1}{2}$ . The same lower bound holds for  $\Delta^-$ . Thus  $M(z)$  is invertible with:  $M(z)^{-1} = \mathcal{O}(h)$  in any fixed matrix norm. From relations (6.18) and (6.19), it follows:

$$(Bq(z, \theta_0, V - W^h) - A)^{-1} = M(z)^{-1} \left( 1 + \mathcal{O} \left( \frac{e^{-\frac{3S_0}{4h}}}{h} \right) \right) = \mathcal{O}(h), \quad (6.20)$$

which is a rewriting of (6.4). The estimate (6.10) of the difference is due to the exponentially small size of  $|u'_{2,3}(a, b) - \tilde{u}'_{2,3}(a, b)|$  stated in (6.17).

**b)** We shall now consider the estimates for  $\gamma_{\mathcal{V}}(e_i)$  with  $i = 2, 3$ ,  $\mathcal{V} = V$  or  $\mathcal{V} = V - W^h$ . Actually it suffices to remember the equations (3.23), (3.24) and the definition of the coefficients (3.25)

$$\gamma_{V-W^h}(\underline{e}_i, z, \theta_0) = c_i u_i = \pm \frac{1}{h^2} u_i, \quad i = 2, 3,$$

where the functions  $u_{2,3}$  do not depend on  $\theta_0$  and are given by (3.24). It suffices to use (6.13) for (6.8) and (6.17) for (6.11). Changing  $\theta_0$  into  $\bar{\theta}_0$  has no effect and  $\bar{z} \in G_h(\lambda^0)$  when  $z \in G_h(\lambda^0)$ .

**c)** The functions  $\gamma_{\mathcal{V}}(\underline{e}_{1,4}, z, \theta_0)$  do not depend on the potential  $\mathcal{V}$ :

$$\gamma(\underline{e}_1, z, \theta_0) = \frac{ie^{\frac{3\theta_0}{2}}}{h\sqrt{ze^{2\theta_0}}} 1_{(b, +\infty)} e^{i\frac{\sqrt{ze^{2\theta_0}}(x-b)}{h}}, \quad \gamma(\underline{e}_4, z, \theta_0) = \frac{ie^{\frac{3\theta_0}{2}}}{h\sqrt{ze^{2\theta_0}}} 1_{(-\infty, a)} e^{-i\frac{\sqrt{ze^{2\theta_0}}(x-a)}{h}},$$

from which (6.12) follows while (6.9) comes from

$$\|\gamma(\underline{e}_i, z, \theta_0)\|_{H^{1,h}(\mathbb{R} \setminus [a,b])}^2 \leq \frac{C}{h \operatorname{Im}(\sqrt{ze^{2\theta_0}})} \leq \frac{C_{a,b,c}}{h^{N_0+1}}, \quad \text{when } z \in G_h(\lambda^0).$$

□

### 6.3 Resolvent estimates

We gather the information given by the Krein formula (6.1) and the control of the finite rank part  $\Upsilon^h(z, \mathcal{V})$  given by Proposition 6.3.

**Proposition 6.5.** *Assume the hypotheses (4.1) (5.4)(5.5)(5.6). Take  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ , and let  $G_h(\lambda^0)$  be the set defined by (6.2).*

**a)** *For  $\mathcal{V} = V$  or  $\mathcal{V} = V - W^h$ , the resolvent  $(H_{\theta_0, \mathcal{V}}(\theta_0) - z)^{-1}$  is estimated by*

$$\forall z \in G_h(\lambda^0), \quad \|(H_{\theta_0, \mathcal{V}}^h(\theta_0) - z)^{-1}\|_{\mathcal{L}(L^2(\mathbb{R}); H^1(\mathbb{R} \setminus \{a, b\}))} \leq \frac{C_{a, b, c}}{h^{N_0+2}}, \quad (6.21)$$

$$\forall z \in G_h(\lambda^0), \quad \|(H_{\theta_0, V-W^h}^h(\theta_0) - z)^{-1}\chi\|_{\mathcal{L}(H^{-1}((a, b)); H^1(\mathbb{R} \setminus \{a, b\}))} \leq \frac{C_{a, b, c, \chi}}{h^{N_0+3}}, \quad (6.22)$$

for any fixed  $\chi \in \mathcal{C}_0^\infty((a, b))$ .

**b)** *The difference of the resolvents equals*

$$\begin{aligned} (H_{\theta_0, V-W^h}^h(\theta_0) - z)^{-1} - (H_{\theta_0, V}^h(\theta_0) - z)^{-1} &= (H_{ND, V-W^h}^h(\theta_0) - z)^{-1} \\ &\quad - (H_{ND, V}^h(\theta_0) - z)^{-1} + R\Upsilon^h(z), \end{aligned} \quad (6.23)$$

with

$$\forall z \in G_h(\lambda^0), \quad \|R\Upsilon^h(z)\|_{\mathcal{L}(L^2(\mathbb{R}); H^1(\mathbb{R} \setminus \{a, b\}))} \leq C_{a, b, c} e^{-\frac{S_0}{4h}}, \quad (6.24)$$

$$\forall z \in G_h(\lambda^0), \quad \|R\Upsilon^h(z)\chi\|_{\mathcal{L}(H^{-1}((a, b)); H^1(\mathbb{R} \setminus \{a, b\}))} \leq C_{a, b, c} e^{-\frac{S_0}{4h}}, \quad (6.25)$$

for any fixed  $\chi \in \mathcal{C}_0^\infty((a, b))$ .

**Proof:** **a)** The formula (6.1) says for  $\mathcal{V} = V$  or  $\mathcal{V} = V - W^h$ :

$$\begin{aligned} (H_{\theta_0, \mathcal{V}}^h(\theta_0) - z)^{-1} &= (H_{ND, \mathcal{V}}^h(\theta_0) - z)^{-1} \\ &\quad - \sum_{i, j, k=1}^4 (Bq(z, \theta_0, \mathcal{V}) - A)_{ij}^{-1} B_{jk} \langle \gamma(\underline{e}_k, \bar{z}, \bar{\theta}_0), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta_0) \\ &= (H_{ND, \mathcal{V}}^h(\theta_0) - z)^{-1} - \Upsilon^h(z, \mathcal{V}). \end{aligned}$$

By Proposition 6.3, actually by (6.4)(6.9) and (6.8), the term  $\Upsilon^h(z, \mathcal{V})$  satisfies with  $N_0 > 1$

$$\begin{aligned} \|\Upsilon^h(z, \mathcal{V})\|_{\mathcal{L}(L^2(\mathbb{R}); H^1(\mathbb{R} \setminus \{a, b\}))} &\leq \frac{C_{a, b, c} h}{\min\{h^{N_0+1}, h^{N_0/2+2}, h^3\}} \times \frac{1}{h} \leq \frac{C_{a, b, c}}{h^{N_0+2}}, \\ \|\Upsilon^h(z, \mathcal{V})\chi\|_{\mathcal{L}(H^{-1}((a, b)); H^1(\mathbb{R} \setminus \{a, b\}))} &\leq \frac{C_{a, b, c, \chi} h}{\min\{h^{N_0+1}, h^{N_0/2+2}, h^3\}} \times \frac{1}{h^2} \leq \frac{C_{a, b, c, \chi}}{h^{N_0+3}}, \end{aligned}$$

for any fixed  $\chi \in \mathcal{C}_0^\infty((a, b))$ .

It remains to estimate the first term. The worst case is for  $\mathcal{V} = V - W^h$  since  $G_h(\lambda^0)$  lies around elements of  $\sigma(H_D^h = -h^2 \Delta_D + V - W^h)$ :

$$(H_{ND, V-W^h}^h(\theta_0) - z)^{-1} = e^{2\theta_0} \left( -h^2 \Delta_{\mathbb{R} \setminus [a, b]}^N - ze^{2\theta_0} \right)^{-1} \oplus (H_D^h - z)^{-1}.$$

According to Lemma A.2 with  $\|f\|_{H^{-1, h}((a, b))} \leq \frac{1}{h} \|f\|_{H^{-1}}$  and  $\|u\|_{H^1((a, b))} \leq \frac{1}{h} \|u\|_{H^{1, h}((a, b))}$ , the inequality

$$\|(H_D^h - z)^{-1}\|_{\mathcal{L}(H^{-1}((a, b)), H_0^1((a, b)))} \leq \frac{C_{a, b, c}}{h^2} \left( \frac{1}{d(z, \sigma(H_D^h))} + 1 \right) \leq \frac{C_{a, b, c}}{h^{N_0+2}},$$

holds for  $z \in G_h(\lambda^0)$ .

The resolvent of the Neumann Laplacian  $\left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N - \zeta\right)^{-1}$  can be written

$$\begin{aligned} \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N - \zeta\right)^{-1} &= \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N + 1\right)^{-1} \left[1 + (1 + \zeta) \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N - \zeta\right)^{-1}\right], \\ \text{with } \left\| \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N + 1\right)^{-1} \right\|_{\mathcal{L}(L^2(\mathbb{R} \setminus [a,b]); H^1(\mathbb{R} \setminus [a,b]))} &\leq \frac{1}{h}, \end{aligned}$$

it is estimated by

$$\left\| \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N - \zeta\right)^{-1} \right\|_{\mathcal{L}(L^2(\mathbb{R} \setminus [a,b]); H^1(\mathbb{R} \setminus [a,b]))} \leq \frac{1}{h} \left[1 + \frac{1 + |\zeta|}{d(\zeta, \mathbb{R}_+)}\right].$$

For  $z \in G_h(\lambda^0)$  and  $\zeta = ze^{2\theta_0}$ , the distance  $d(ze^{2\theta_0}, \mathbb{R}_+)$ , is bounded from below by  $Ch^{N_0}$ . Hence we get

$$\left\| \left(-h^2 \Delta_{\mathbb{R} \setminus [a,b]}^N - ze^{2\theta_0}\right) \right\|_{\mathcal{L}(L^2(\mathbb{R} \setminus [a,b]); H^1(\mathbb{R} \setminus [a,b]))} \leq \frac{C_{a,b,c}}{h^{N_0+1}}.$$

Putting all together gives (6.21) and (6.22).

b) For the difference of resolvents, it suffices to notice that

$$R\Upsilon^h(z) = \Upsilon^h(z, V) - \Upsilon^h(z, V - W^h).$$

Hence it is the difference of trilinear quantities of which every factor is estimated by  $\frac{1}{h^{3N_0}}$  with variations bounded by  $\frac{C_{a,b,c}}{h} e^{-\frac{S_0}{2h}}$ . This ends the proof.  $\square$

## 7 Adiabatic evolution

We consider now a time-dependent real valued potential  $V(t) - W^h(t) = V(t) - W_1^h(t) - W_2^h(t)$  supported in  $[a, b]$  with

$$W_1^h(x, t) = \sum_{j_1=1}^{M_1} w_{j_1}\left(\frac{x - x_{j_1,1}}{h}, t\right), \quad W_2^h(t) = \sum_{j_2=1}^{M_2} \alpha_{j_2}(t) h \delta(x - x_{j_2,2}), \quad \alpha_{j_2}(t) > 0, \quad (7.1)$$

where the  $x_j$ 's are fixed (independent of  $h$ ) distinct points of  $(a, b)$  and the supports  $\text{supp } w_{j_1}$  are contained in a fixed compact set. The functions  $V(\cdot, t)$ ,  $w_{j_1}(\cdot, t)$ ,  $\alpha_{j_2}(t)$  are possibly  $h$ -dependent  $C^K$  functions with a uniform control of the derivatives and which impose a uniform control of (4.1)(5.4)(5.5)(5.6). Namely we assume that for some  $\lambda^0(t)$  the estimates

$$\max_{\substack{t \in [0, T] \\ 0 \leq k \leq K \\ 0 \leq j_1 \leq M_1 \\ 0 \leq j_2 \leq M_2}} \|\partial_t^k V(t)\|_{L^\infty} + \|\partial_t^k w_{j_1}(t)\|_{L^\infty} + |\partial_t^k \alpha_{j_2}(t)| + |\partial_t^k \lambda^0(t)| \leq \frac{1}{c}, \quad (7.2)$$

$$\forall x \in [a, b], \quad c \leq \lambda^0(t) \leq V(x, t) - c, \quad (7.3)$$

hold for all  $t \in [0, T]$ . Actually, the regularity of  $\lambda^0(t)$  can be deduced from the other assumptions possibly by replacing it initial guess by the mean energy value  $\frac{1}{\ell} \text{Tr} [H_D^h(t) \Pi_0(t)]$  with  $\Pi_0(t) = \frac{1}{2i\pi} \int_{|z - \lambda_0(t)| = \frac{2h}{c}} (z - H_D^h(t))^{-1} dz$ .

This  $\lambda^0(t)$  is moreover assumed to be the center of a cluster of eigenvalues of the Dirichlet Hamiltonian  $H_D^h(t) = -h^2 \Delta_D + V(t) - W^h(t)$  on  $(a, b)$ : There exist  $\lambda_1^h(t), \dots, \lambda_\ell^h(t) \in \sigma(H_D^h(t))$  such that

$$d(\lambda^0(t), \sigma(H_D^h(t)) \setminus \{\lambda_1^h(t), \dots, \lambda_\ell^h(t)\}) \geq c, \quad (7.4)$$

$$\max_{1 \leq j \leq \ell} |\lambda_j^h(t) - \lambda^0(t)| \leq \frac{h}{c}. \quad (7.5)$$

The operator  $H_{\theta_0, V(t)-W^h(t)}^h(\theta_0)$  is studied here with

$$\theta_0 = ih^{N_0}, \quad N_0 > 1.$$

According to Proposition 6.1 and Definition 6.2, the complex domain  $G_h(\lambda_0(t))$  surrounds  $\ell$  eigenvalues  $z_1^h(t), \dots, z_\ell^h(t)$  of  $H_{\theta_0, V(t)-W^h(t)}^h(\theta_0)$  and its distance to the spectrum remains uniformly bounded from below

$$\min_{t \in [0, T]} d(G_h(\lambda_0(t)), \sigma(H_{\theta_0, V(t)-W^h(t)}^h(\theta_0))) \geq \frac{1}{C_{a,b,c}} h^{N_0}.$$

The spectral projection associated with the cluster of eigenvalues  $\{z_1^h, \dots, z_\ell^h\}$  is given by

$$P_0(t) = \frac{1}{2i\pi} \int_{\Gamma^h(t)} (z - H_{\theta_0, V(t)-W^h(t)}^h(\theta_0))^{-1} dz, \quad (7.6)$$

where  $\Gamma^h(t)$  is a contour contained in  $G_h(\lambda^0(t))$ .

When  $K \geq 1$ , the parallel transport  $\Phi_0(t, s)$ ,  $t, s \in [0, T]$ , associated with  $(P_0(t))_{t \in [0, T]}$  is given by

$$\begin{cases} \partial_t \Phi_0 + [P_0, \partial_t P_0] \Phi_0 = 0 \\ \Phi_0(t = s, s) = \text{Id} \end{cases} \quad (7.7)$$

is well defined and satisfies

$$\forall s, t \in [0, T], \quad P_0(t) \Phi_0(t, s) = \Phi_0(t, s) P_0(s).$$

The time-scale is given by the parameter

$$\varepsilon = e^{-\frac{\tau}{h}}, \quad \text{with } \tau > 0 \text{ fixed.}$$

When the assumed regularity is large enough,  $K \geq 2$ , Proposition 3.7-d). the Cauchy problem

$$\begin{cases} i\varepsilon \partial_t u = H_{\theta_0, V(t)-W^h(t)}^h(\theta_0) u, & t \geq s, \\ u(t = s) = u_s \end{cases} \quad (7.8)$$

defines a dynamical system  $U^\varepsilon(t, s)$ ,  $0 \leq s \leq t \leq T$ , of contractions on  $L^2(\mathbb{R})$ .

**Theorem 7.1.** Assume (7.2)(7.4)(7.3)(7.5) with  $K \geq 2$  and take  $\theta_0 = ih^{N_0}$ ,  $N_0 > 1$ ,  $\varepsilon = e^{-\frac{\tau}{h}}$ ,  $\tau > 0$ . Let  $P_0(t)$  be the spectral projection (7.6), let  $r$  belong to  $\mathcal{C}^0([0, T]; L^2(\mathbb{R}))$  and let  $r_s$  belong to  $L^2(\mathbb{R})$ . For  $s \in [0, T]$  take an initial data  $u_s \in L^2(\mathbb{R})$  such that  $P_0(s)u_s = u_s$ . Then the solutions  $u^h$  and  $v^h$  to the Cauchy problems

$$\begin{cases} i\varepsilon \partial_t u^h = H_{\theta_0, V(t)-W^h(t)}^h(\theta_0) u^h + r(t), & t \geq s, \\ u^h(t = s) = u_s + r_s \end{cases} \quad (7.9)$$

and

$$\begin{cases} i\varepsilon \partial_t v^h = \Phi_0(s, t) P_0(t) (H_{\theta_0, V(t)-W^h(t)}^h(\theta_0)) P_0(t) \Phi_0(t, s) v^h, & t \geq s \\ v^h(t = s) = u_s, \end{cases}$$

satisfy

$$\max_{t \in [s, T]} \|u^h(t) - \Phi_0(t, s) v^h(t)\| \leq C_{a,b,c,\tau,T,\delta} \left[ \varepsilon^{1-\delta} \|u_s\| + \|r_s\| + \frac{1}{\varepsilon} \max_{t \in [s, T]} \|r(t)\| \right]. \quad (7.10)$$

**Remark 7.2.** The estimate with the source term  $r(t)$  can be improved if  $P(t)r(t) = r(t)$  after reconsidering the proof of Corollary B.2 in the Appendix (possibly with a higher order starting approximation with  $K \leq 2$ ). Nevertheless the accuracy of the result may depend on the assumptions for  $r(t)$ . We prefer to postpone this kind of improvement to a subsequent work when hypotheses for the source term are naturally introduced.

**Proof:** **a)** When  $u_{00}^h(t)$  denotes the solution to (7.8) associated with  $r_s = 0$  and  $r \equiv 0$ , the contraction property of  $U^\varepsilon(t, s)$  implies

$$\max_{t \in [s, T]} \|u(t) - u_{00}(t)\| \leq \|r_s\| + \frac{1}{\varepsilon} \max_{t \in [s, T]} \|r(t)\|.$$

Hence, we can forget the remainder terms and simply prove the estimate (7.10) when  $r_s = 0$  and  $r \equiv 0$ .

**b)** We consider the operator  $A^\varepsilon(t) = \frac{1}{i}(H_{\theta_0, V(t)-W^h(t)}(\theta_0) - \lambda^0(t))$  and we notice that the domain

$$\frac{1}{i}(G_h(\lambda^0(t)) - \lambda^0(t)) = \left\{ \frac{1}{i}(z - \lambda^0(t)), \quad z \in G_h(\lambda_0(t)) \right\}$$

contains the contour

$$\Gamma_\varepsilon = \frac{1}{i} \{ \Gamma^h(t) - \lambda^0(t) \},$$

which can be chosen independent of  $t \in [0, T]$ . Then the projection  $P_0(t)$  is nothing but

$$P_0(t) = \frac{1}{2i\pi} \int_{\Gamma_\varepsilon} (z - A^\varepsilon(t))^{-1} dt.$$

Hence it suffices to verify the estimates of  $\partial_t^k(z - A^\varepsilon(t))^{-1}$  for  $k \leq K+1$  and  $t \in [0, T]$  in order to apply Theorem B.1 and additionally the uniform boundedness of  $\|P_0(t)\|$  and  $\|\partial_t P_0(t)\|$  in order to use its Corollary B.2.

Like in Appendix B, we use the notation  $g(\varepsilon) = \tilde{\mathcal{O}}(\varepsilon^N)$  in order to summarize

$$\forall \delta > 0, \exists C_{g,\delta} > 0, \quad |g(\varepsilon)| \leq C_{g,\delta} \varepsilon^{N-\delta}.$$

For  $z \in \Gamma_\varepsilon$ , the  $k$ -th derivative of  $(z - A^\varepsilon(t))^{-1}$  has the form

$$\begin{aligned} \partial_t^k(z - A^\varepsilon(t))^{-1} = & \sum_{\substack{j_1 + \dots + j_m = k \\ j_i \geq 1}} c_{j_1, \dots, j_m} (z - A^\varepsilon)^{-1} [\partial_t^{j_1}(-iV + iW^h)](z - A^\varepsilon)^{-1} \dots \\ & \dots [\partial_t^{j_m}(-iV + iW^h)](z - A^\varepsilon)^{-1}, \end{aligned}$$

where the numbers  $c_{j_1, \dots, j_\ell}$  are universal coefficients.

Remember

$$\|\partial_t^j V(t)\|_{\mathcal{L}(L^2(\mathbb{R}))} \leq \frac{1}{c},$$

the support condition

$$\partial_t^j W(t) = \chi(x) \left[ \partial_t^j W(t) \right] \chi(x)$$

with  $\chi \in \mathcal{C}_0^\infty((a, b))$ , which entails

$$\|\partial_t^j W(t)\|_{\mathcal{L}(H_0^1((a, b)); H^{-1}((a, b)))} \leq \frac{1}{c}.$$

Hence the resolvent estimates of Proposition 6.5 imply

$$\max_{z \in \Gamma_\varepsilon, k \leq K+1, t \in [0, T]} \|\partial_t^k(z - A^\varepsilon(t))^{-1}\| \leq \frac{C_{a,b,c}}{h^{k(N_0+3)}} = \tilde{\mathcal{O}}(\varepsilon^0). \quad (7.11)$$

Meanwhile the length  $|\Gamma_\varepsilon|$  is bounded by  $\mathcal{O}(1)$  and therefore the conclusions of Theorem B.1 are valid.

Now comes the final points, which are the uniform boundedness of  $\|P_0(t)\|$  and  $\|\partial_t P_0(t)\|$ , in order to refer to the more accurate version of Corollary B.2.

**c)** For  $P_0(t)$ , we write

$$P_0(t) = \frac{1}{2i\pi} \int_{\Gamma_\varepsilon} (z - A^\varepsilon(t))^{-1} dz = \frac{1}{2i\pi} \int_{\Gamma^h(t)} (z - H_{\theta_0, V(t)-W^h(t)}(\theta_0))^{-1} dz,$$

and we use the formula (6.23) in the form

$$(H_{\theta_0, V-W^h}^h(\theta_0) - z)^{-1} - (H_D^h - z)^{-1} = e^{2\theta_0}(-h^2 \Delta_{\mathbb{R} \setminus [a, b]}^N - ze^{2\theta_0})^{-1} \\ + (H_{\theta_0, V}^h(\theta_0) - z)^{-1} - (H_{ND, V}^h(\theta_0) - z)^{-1} + R\Upsilon^h(z). \quad (7.12)$$

The right-hand side is the sum of three holomorphic terms in the interior of  $\Gamma^h(t)$  and of an exponentially small term according to (6.24). We obtain

$$P_0(t) = \frac{1}{2i\pi} \int_{\Gamma^h(t)} (z - H_D^h)^{-1} dz + \mathcal{O}(e^{-\frac{S_0}{4h}}) = \Pi_0(t) + \mathcal{O}(e^{-\frac{S_0}{4h}}),$$

where  $\Pi_0(t)$  is the orthogonal spectral projector associated with  $\{\lambda_1^h(t), \dots, \lambda_\ell^h(t)\} \subset \sigma(H_D^h(t))$  with norm  $\|\Pi_0(t)\| \leq 1$ .

**d)** For  $\partial_t P_0(t)$ , we use

$$\partial_t(z - H_{\theta_0, V-W^h}(\theta_0))^{-1} = (z - H_{\theta_0, V-W^h}(\theta_0))^{-1}(\partial_t V - \partial_t W^h)(z - H_{\theta_0, V-W^h}(\theta_0))^{-1}.$$

From (7.12), we get

$$(H_{\theta_0, V-W^h}(\theta_0) - z)^{-1} 1_{[a, b]} - (H_D^h - z)^{-1} 1_{[a, b]} \\ = 0 + \Upsilon^h(z, V) 1_{[a, b]} + R\Upsilon^h(z) 1_{[a, b]} \\ = \sum_{i, j=1}^4 \sum_{k=2}^3 (Bq(z, \theta_0, V) - A)_{ij}^{-1} B_{jk} \langle \gamma(\underline{e}_k, \bar{z}, \bar{\theta}_0), \cdot \rangle_{L^2(\mathbb{R})} \gamma(\underline{e}_i, z, \theta_0) + R\Upsilon^h(z) 1_{[a, b]},$$

where the first term of the right-hand side is holomorphic inside  $\Gamma^h(t)$  and the last term is exponentially small according to (6.24) and (6.25). A symmetric writing holds for  $1_{[a, b]}(z - H_{\theta_0, V-W^h}(\theta_0))^{-1}$ . Hence the derivative  $\partial_t P_0(t)$  is the sum of several terms:

$$\frac{1}{2i\pi} \int_{\Gamma^h(t)} (z - H_D^h)^{-1} (\partial_t V - \partial_t W^h)(z - H_D^h)^{-1} dz = \partial_t \Pi_0(t) \\ = \frac{1}{2i\pi} \int_{|z - \lambda^0(t)| = c/2} (z - H_D^h)^{-1} (\partial_t V - \partial_t W^h)(z - H_D^h)^{-1} dz, \quad (7.13)$$

$$- \frac{1}{2i\pi} \int_{\Gamma^h(t)} \Upsilon^h(z, V) 1_{[a, b]} (\partial_t V - \partial_t W^h)(z - H_D^h) dz \\ = - \sum_{j'=1}^{\ell} \Upsilon^h(\lambda_{j'}^h, V) (\partial_t V - \partial_t W^h) |\Phi_{j'}^h\rangle \langle \Phi_{j'}^h|, \quad (7.14)$$

$$- \frac{1}{2i\pi} \int_{\Gamma^h(t)} (z - H_{\theta_0, V-W^h}(\theta_0))^{-1} (\partial_t V - \partial_t W^h) R\Upsilon^h(z) dz, \quad (7.15)$$

plus another term symmetric to (7.14).

The first one (7.13) is uniformly bounded because

- $\|(z - H_D^h)^{-1}\|_{\mathcal{L}(L^2)}$  is uniformly bounded when  $|z - \lambda^0(t)| = \frac{c}{2}$  according to Hypothesis (7.4)(7.5) with  $\|\partial_t V\|_{L^\infty} + \|\partial_t W_1^h\|_{L^\infty} \leq \frac{1}{c}$ ,
- $\|(z - H_D^h)^{-1}\|_{\mathcal{L}(L^2, H_0^{1, h})}$  is uniformly bounded when  $|z - \lambda^0(t)| = \frac{c}{2}$  according to (7.4)(7.5) and (A.1) in Lemma A.2 with  $\|\partial_t W_2^h\|_{\mathcal{M}_b} \leq \frac{h}{c}$ .

The last one (7.15) is  $\mathcal{O}(e^{-\frac{S_0}{8h}})$  owing to (6.24)(6.25) for  $R\Upsilon^h(z)$  and owing to (6.21)(6.22) for  $(z - H_{\theta_0, V-W^h}(\theta_0))^{-1}$ .

For the middle term (7.14) and its symmetric counterpart, first consider for  $k = 2, 3$  and  $j' \in \{1, \dots, \ell\}$

$$\langle \gamma(\underline{e}_k, \bar{z}, \bar{\theta}_0), (\partial_t V - \partial_t W^h) \Phi_{j'}^h \rangle = \pm \frac{1}{h^2} \langle \tilde{u}_k, (\partial_t V - \partial_t W^h) \Phi_{j'}^h \rangle,$$



where  $\tilde{u}_2$  and  $\tilde{u}_3$  are recalled in Lemma 6.4. The exponential decay estimates for  $\tilde{u}_{2,3}$  stated in (6.13)(6.14) and the one for  $\Phi_j^h$ , stated in Proposition 4.1-ii) combined with  $\|\partial_t(V - W^h)\|_{\mathcal{M}_b} \leq \frac{1}{c}$  imply that the scalar product is smaller than  $e^{-\frac{S_0}{2h}}$ . Since the other factors of (7.14) are bounded by  $Ch$  or  $\frac{C}{h^{N_0}}$ , we conclude (7.14) and its symmetric counterpart are smaller than  $e^{-\frac{S_0}{4h}}$ .  $\square$

## A Parameter dependent elliptic estimates on the interval $[a, b]$

We gather here elementary  $h$ -dependent estimates for the elliptic operator  $-h^2\Delta + \mathcal{V}$  on the interval  $(a, b)$ .

### A.1 Dirichlet problem

It is convenient to use the  $h$ -dependent  $H^k$ -norms

$$\|u\|_{H^{k,h}}^2 = \sum_{\alpha \leq k} \|(h\partial_x)^\alpha u\|_{L^2}^2,$$

for  $k \in \mathbb{N}$ . The estimates with the standard  $H^k$ ,  $k \in \mathbb{N}$ , can be recovered after

$$\|u\|_{H^k} \leq \frac{1}{h^k} \|u\|_{H^{k,h}}.$$

For  $k = -1$ , the  $h$ -dependent norm on  $H^{-1}((a, b)) = [H_0^1((a, b))]'$  is

$$\|f\|_{H^{-1,h}((a,b))} = \sup_{u \in H_0^1((a,b))} \frac{|\langle f, u \rangle|}{\|u\|_{H^{1,h}((a,b))}},$$

with now  $\|f\|_{H^{-1,h}((a,b))} \leq \frac{1}{h} \|f\|_{H^{-1}((a,b))}$ . We will note  $H_0^{1,h}((a, b))$  the space  $H_0^1((a, b))$  equipped with the  $H^{1,h}$  norm.

**Lemma A.1.** *There exists a constant  $C > 0$  such that*

$$\forall u \in \mathcal{C}^\infty([0, h]), \quad |u(0)| \leq \frac{C}{h^{1/2}} \|u\|_{H^{1,h}((0,h))}, \quad \text{resp. } |u'(0)| \leq \frac{C}{h^{3/2}} \|u\|_{H^{2,h}((0,h))},$$

and the inequality extends to  $H^1((0, h))$  (resp.  $H^2((0, h))$ ).

**Proof:** The second estimate is simply a consequence of the first one after replacing  $u$  with  $hu'$ . The first estimate is simply the usual estimate  $|v(0)| \leq C\|v\|_{H^1((0,1))}$  applied with  $v(x) = u(hx)$ .  $\square$

**Lemma A.2.** *Let  $\mathcal{V}_1 \in L^\infty((a, b))$  and  $\mathcal{V}_2 \in \mathcal{M}_b((a, b))$  be real valued with  $\text{supp } \mathcal{V}_2 \subset \subset (a, b)$  and*

$$\|\mathcal{V}_1\|_{L^\infty} \leq \frac{1}{c}, \quad \|\mathcal{V}_2\|_{\mathcal{M}_b} \leq \frac{h}{c}.$$

*Then the Dirichlet Hamiltonian  $H_D^h = -h^2\Delta + \mathcal{V}_1 + \mathcal{V}_2$  defined with the form domain  $H_0^1((a, b))$ , satisfies the resolvent estimate*

$$\forall z \notin \sigma(H_D^h), \quad \|(H_D^h - z)^{-1}\|_{\mathcal{L}(H^{-1,h}((a,b)); H_0^{1,h}((a,b)))} \leq C_{a,b,c} [1 + |z|]^2 \left(1 + \frac{1}{d(z, \sigma(H_D^h))}\right). \quad (\text{A.1})$$

*When  $f \in L^2((a, b))$  and  $z \notin \sigma(H_D^h)$  the traces  $u'(a)$  and  $u'(b)$  of  $u = (H_D^h - z)^{-1}f$  are well defined with*

$$|u'(a)| + |u'(b)| \leq \frac{C'_{a,b,c} [1 + |z|]^2}{h^{5/2}} \left(1 + \frac{1}{d(z, \sigma(H_D^h))}\right) \|f\|_{L^2}. \quad (\text{A.2})$$

**Proof:** From the Gagliardo-Nirenberg estimate  $|u(x)|^2 \leq \frac{C_{a,b}}{h} \|hu'\|_{L^2} \|u\|_{L^2}$  with  $\|\mathcal{V}_2\|_{\mathcal{M}_b} \leq \frac{h}{c}$ , the term  $\langle u, \mathcal{V}_2 u \rangle$  in the variational formulation is bounded by

$$|\langle u, \mathcal{V}_2 u \rangle| \leq \frac{C_{a,b}}{c} \|hu'\|_{L^2} \|u\|_{L^2} \leq \frac{1}{2} \|hu'\|_{L^2}^2 + \frac{C_{a,b}^2}{2c^2} \|u\|_{L^2}^2.$$

With

$$\forall u \in H_0^1((a, b)), \quad \langle u, H_D^h u \rangle + C \|u\|_{L^2}^2 \geq \frac{1}{2} \|hu'\|_{L^2}^2 + \left( C - \|\mathcal{V}_1\|_{L^\infty} - \frac{C_{a,b}^2}{2c^2} \right) \|u\|_{L^2}^2,$$

the operator  $H_D^h + C$  is bounded from below by  $-\frac{h^2}{2} \Delta_D + \frac{C}{2}$  when  $C \geq \frac{2}{c} + \frac{C_{a,b}^2}{c^2} \geq \|\mathcal{V}_1\|_{L^\infty} + \frac{C_{a,b}^2}{c^2}$ . Lax-Milgram theorem then says

$$\|(H_D^h + C)^{-1} f\|_{H_0^{1,h}((a,b))} \leq C_{a,b,c} \|f\|_{H^{-1,h}((a,b))}.$$

From the iterated first resolvent formula,

$$(H_D^h - z)^{-1} = (H_D^h + C)^{-1} + (C + z)(H_D^h + C)^{-2} + (C + z)^2 (H_D^h + C)^{-1} (H_D^h - z)^{-1} (H_D^h + C)^{-1},$$

we deduce (A.1).

It contains also the estimate  $\|(H_D^h + C)^{-1}\|_{\mathcal{L}(L^2((a,b)); H_0^{1,h}((a,b)))} \leq \frac{C_{a,b,c}}{h}$  and with

$$(H_D^h - z)^{-1} = (H_D^h + C)^{-1} + (C + z)(H_D^h + C)^{-1} (H_D^h - z)^{-1},$$

this yields

$$\|(H_D^h - z)^{-1}\|_{\mathcal{L}(L^2((a,b)); H_0^{1,h}((a,b)))} \leq \frac{C_{a,b,c} [1 + |z|]}{h} \left( 1 + \frac{1}{d(z, \sigma(H_D^h))} \right).$$

When  $u = (H_D^h - z)^{-1} f$  with  $f \in L^2((a, b))$ , writing the equation in  $[a, a + h]$  and  $[b - h, b]$  in the form  $-h^2 u'' = f - (\mathcal{V}_1 - z)u$  implies

$$\|u\|_{H^{2,h}((a, a+h) \cup (b-h, b))} \leq \frac{C_{a,b,c} [1 + |z|]^2}{h} \left( 1 + \frac{1}{d(z, \sigma(H_D^h))} \right) \|f\|_{L^2}.$$

Lemma A.1 is applied to  $u(a + \cdot)$  and  $u(b - \cdot)$  in order to get (A.2).  $\square$

## A.2 Agmon estimate

The next estimate is the usual energy estimate with exponential weights (see [2][28]).

**Lemma A.3.** *Let  $(\alpha, \beta)$  be an open interval,  $V \in L^\infty((\alpha, \beta))$ ,  $z \in \mathbb{C}$  and  $\varphi \in W^{1,\infty}((\alpha, \beta); \mathbb{R})$ . Denote by  $P$  the Schrödinger operator  $P := -h^2 d^2/dx^2 + V$ . Then for any  $u_1, u_2$  in  $H^1((\alpha, \beta))$  such that  $u_1''$  is a bounded measure in  $(\alpha, \beta)$  and locally  $L^2$  around  $\alpha$  and  $\beta$ , the identity*

$$\begin{aligned} \int_\alpha^\beta \bar{u}_2 e^{2\frac{\varphi}{h}} (P - z) u_1 dx &= \int_\alpha^\beta \overline{h v_2'} h v_1' dx + \int_\alpha^\beta (V - z - \varphi'^2) \bar{v}_2 v_1 dx \\ &+ \int_\alpha^\beta h \varphi' (\bar{v}_2 v_1' - \bar{v}_2' v_1) dx \\ &+ h^2 \left( e^{2\frac{\varphi(\alpha)}{h}} \bar{u}_2 u_1'(\alpha) - e^{2\frac{\varphi(\beta)}{h}} \bar{u}_2 u_1'(\beta) \right) \end{aligned} \quad (\text{A.3})$$

holds by setting  $v_j := e^{\varphi/h} u_j$  for  $j = 1, 2$ .

This identity is obtained after conjugation of  $h d/dx$  by  $e^{\varphi/h}$  and integration by parts. The weak regularity assumptions can be checked after regularizing individually  $u_1$ ,  $u_2$ ,  $\varphi$  or  $V$ . In [46] it was even considered with possible jumps of the derivative  $u_1'$  at  $\alpha$  and  $\beta$ , which are here removed by the simplifying condition that  $u_1$  is locally  $H^2$  around  $\alpha$  and  $\beta$  (Jump conditions already occur at the ends of our intervals).

## B Variation on adiabatic evolutions.

We shall consider a family of contraction semigroup generators  $(A^\varepsilon(s))_{s \in [0, +\infty)}$  which fulfill the two next properties.

- The Cauchy problem

$$\begin{cases} i\varepsilon \partial_t u_t = iA^\varepsilon(t)u_t \\ u_{t=0} = u_0 \end{cases} \quad (\text{B.1})$$

admits a unique strong solution with  $u_t \in D(A^\varepsilon(t))$  for all  $t \geq 0$  as soon as  $u_0 \in D(A^\varepsilon(0))$ . The corresponding dynamical system of contractions is denoted  $(S^\varepsilon(t, s))_{t \geq s}$  with the property  $S^\varepsilon(t, s)D(A^\varepsilon(s)) \subset D(A^\varepsilon(t))$ .

- The resolvent  $(z - iA^\varepsilon(s))^{-1}$  defines  $\mathcal{C}^{K+1}([0, +\infty); \mathcal{L}(\mathcal{H}))$  function for some  $z \in \mathbb{C}$  and that there exists a contour  $\Gamma_\varepsilon \subset \mathbb{C}$  independent of  $s \in [0, T]$ , such that

$$|\Gamma_\varepsilon| + \max_{z \in \Gamma_\varepsilon, s \in [0, T]} \|\partial_s^k (z - A^\varepsilon(s))^{-1}\| \leq \frac{a_{k, \delta}}{\varepsilon^\delta},$$

for any  $k \in \{0, \dots, K+1\}$ ,  $K \in \mathbb{N}$ , any  $\delta \in (0, \delta_0)$  and any  $\varepsilon \in (0, \varepsilon_0)$ .

**Notation:** We shall use the notation  $g(\varepsilon) = \tilde{\mathcal{O}}(\varepsilon^N)$  for any  $N \in \mathbb{Z}$  in order to summarize

$$\forall \delta > 0, \exists C_{g, \delta} > 0, \quad |g(\varepsilon)| \leq C_{g, \delta} \varepsilon^{N-\delta}.$$

For example, the previous assumption can be written

$$|\Gamma_\varepsilon| = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{and} \quad \max_{k \leq K+1, z \in \Gamma_\varepsilon, s \in [0, T]} \|\partial_s^k (z - A^\varepsilon(s))^{-1}\| = \tilde{\mathcal{O}}(\varepsilon^0). \quad (\text{B.2})$$

The spectral projection  $P_0(t) = E_0(t)$  is defined as a contour integral along  $\Gamma_\varepsilon$  of the resolvent  $(z - A^\varepsilon(t))^{-1}$ . Correction terms  $E_j(t)$ ,  $1 \leq j \leq K$  are then constructed by induction. The finite sequence  $(E_j^\varepsilon)_{0 \leq j \leq K}$  is defined according to

$$E_0^\varepsilon(s) = P_0^\varepsilon(s) = \frac{1}{2i\pi} \int_{\Gamma_\varepsilon} (z - A^\varepsilon(s))^{-1} dz, \quad Q_0^\varepsilon(s) = 1 - P_0^\varepsilon(s), \quad (\text{B.3})$$

$$S_j^\varepsilon(s) = \sum_{m=1}^{j-1} E_m^\varepsilon(s) E_{j-m}^\varepsilon(s), \quad \text{if } 2 \leq j \leq K, \quad S_0^\varepsilon = S_1^\varepsilon = 0, \quad (\text{B.4})$$

$$E_j^\varepsilon(s) = \frac{i}{2\pi} \int_{\Gamma_\varepsilon} R^\varepsilon \{ Q_0^\varepsilon(s) \partial_s E_{j-1}^\varepsilon(s) P_0^\varepsilon(s) - P_0^\varepsilon(s) \partial_s E_{j-1}^\varepsilon(s) Q_0^\varepsilon(s) \} R^\varepsilon dz \quad (\text{B.5})$$

$$+ S_j^\varepsilon(s) - 2P_0^\varepsilon(s) S_j^\varepsilon(s) P_0^\varepsilon(s), \quad \text{with } R^\varepsilon = (z - A^\varepsilon(s))^{-1}. \quad (\text{B.6})$$

**Theorem B.1.** *There exists a  $\mathcal{C}^1$ -projection valued function  $(P^\varepsilon(s))_{s \geq 0}$  such that the relations and estimates*

$$P^\varepsilon(s)P^\varepsilon(s) = P^\varepsilon(s) \quad , \quad P^\varepsilon(s) \in \mathcal{L}(\mathcal{H}, D(A^\varepsilon(s))), \quad (\text{B.7})$$

$$P^\varepsilon(s) = \sum_{j=0}^K \varepsilon^j E_j^\varepsilon(s) + \tilde{\mathcal{O}}(\varepsilon^{K+1}) \quad \text{with } E_j^\varepsilon(s) = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{in } \mathcal{L}(\mathcal{H}), \quad (\text{B.8})$$

$$P^\varepsilon(s)A^\varepsilon(s) = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{and} \quad A^\varepsilon(s)P^\varepsilon(s) = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{in } \mathcal{L}(\mathcal{H}), \quad (\text{B.9})$$

$$i\varepsilon \partial_s P^\varepsilon(s) - [iA^\varepsilon(s), P^\varepsilon(s)] = \tilde{\mathcal{O}}(\varepsilon^{K+1}) \quad \text{in } \mathcal{L}(\mathcal{H}), \quad (\text{B.10})$$

hold with uniform constants with respect to  $s, t \in [0, T]$  for any fixed  $T < +\infty$ . Moreover for  $K \geq 1$ , if  $u_s = P^\varepsilon(s)u_s$  then  $u^\varepsilon(t) = S^\varepsilon(t, s)u_s$  satisfies

$$\sup_{s \leq t \leq T} \|u^\varepsilon(t) - v^\varepsilon(t)\| = \tilde{\mathcal{O}}(\varepsilon^K), \quad (\text{B.11})$$

$$\text{with} \quad v^\varepsilon(t) = P^\varepsilon(t)v^\varepsilon(t), \quad (\text{B.12})$$

$$\text{and} \quad \begin{cases} i\varepsilon \partial_t v^\varepsilon - i\varepsilon (\partial_t P^\varepsilon(t))v^\varepsilon = P^\varepsilon(t)(iA^\varepsilon(t))P^\varepsilon(t)v^\varepsilon, & \text{for } t \geq s, \\ v^\varepsilon(t=s) = u_s. \end{cases} \quad (\text{B.13})$$

The proof of this theorem follows the lines of [43]. For the sake of completeness, we check that the computations are still valid in the non self-adjoint unbounded case (bounded self-adjoint generators have been considered in [44] [55]) and that the  $\tilde{\mathcal{O}}(\varepsilon^0)$  estimates can be propagated in the induction process like the uniform constants in [43]. Part of the analysis could be pushed further in the spirit of [35] in order to get  $\mathcal{O}(e^{-\frac{\varepsilon}{\varepsilon}})$  error under analyticity assumptions but the techniques developed by A. Joye in this article should be adapted in order to work with a  $\varepsilon$ -dependent gap or with  $\tilde{\mathcal{O}}(\varepsilon^0)$  resolvent estimates, maybe by including all the additional information provided by our model.

As it is stated, the previous result cannot be used for  $K = 0$  and is not formulated as usual with a reduced evolution on the fixed space  $\text{Ran} P^\varepsilon(s)$  after introducing the parallel transport associated with the  $\mathcal{C}^1$  family  $(P^\varepsilon(t))_{t \geq s}$ . Actually both problems can be solved at the first order with an additional uniform boundedness assumption on  $E_0^\varepsilon(t)$  and  $\partial_t E_0^\varepsilon(t)$ . This will be obtained as a corollary of Theorem B.1, used with  $K = 1$  before reconsidering the case  $K = 0$ . The parallel transport  $\Phi_0^\varepsilon(t', s')$ , associated with  $(E_0^\varepsilon(t))_{t \in [0, T]}$ , is defined for  $t', s' \in [0, T]$  by

$$\begin{cases} \partial_{t'} \Phi_0^\varepsilon + [E_0^\varepsilon, \partial_{t'} E_0^\varepsilon] \Phi_0^\varepsilon = 0 \\ \Phi_0^\varepsilon(t' = s', s') = \text{Id} \end{cases} \quad (\text{B.14})$$

and the uniform boundedness of  $\Phi_0^\varepsilon(t', s')$  is inherited from the one of  $E_0^\varepsilon(t)$  and  $\partial_t E_0^\varepsilon(t)$ .

**Corollary B.2.** *With the hypotheses of Theorem B.1 with  $K \geq 1$ , assume additionally that the projector  $E_0^\varepsilon(s)$  defined in (B.3) and its derivative  $\partial_s E_0^\varepsilon(s)$  are uniformly bounded continuous functions:*

$$\exists C > 0, \forall \varepsilon \in (0, \varepsilon_0), \quad \max_{s \in [0, T]} \|E_0^\varepsilon(s)\| + \|\partial_s E_0^\varepsilon(s)\| \leq C.$$

Then for  $K \geq 1$  and when  $u_s = E_0^\varepsilon(s)u_s$ , the solution  $u^\varepsilon(t) = S^\varepsilon(t, s)u_s$  to (B.1) satisfies

$$\sup_{s \leq t \leq T} \|u^\varepsilon(t) - \Phi_0^\varepsilon(t, s)w^\varepsilon(t)\| = \tilde{\mathcal{O}}(\varepsilon)\|u_s\|, \quad (\text{B.15})$$

where  $\Phi_0^\varepsilon(t', s')$  is the parallel transport defined for  $t', s' \in [0, T]$  by (B.14) and  $w^\varepsilon \in E_0^\varepsilon(s)\mathcal{H}$  solves the Cauchy problem

$$\begin{cases} i\varepsilon \partial_t w^\varepsilon = \Phi_0^\varepsilon(s, t)E_0^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t)\Phi_0^\varepsilon(t, s)w^\varepsilon = E_0^\varepsilon(s)\Phi_0^\varepsilon(s, t)(iA^\varepsilon(t))\Phi_0^\varepsilon(t, s)E_0^\varepsilon(s)w^\varepsilon \\ w^\varepsilon(t = s) = u_s. \end{cases}$$

Theorem B.1 and Corollary B.2 are proved in several steps. We start with uniform estimates for the  $E_j$ 's.

**Proposition B.3.** *For all  $j \in \{0, \dots, K\}$ , and any  $T \in \mathbb{R}_+$ , the  $\mathcal{L}(\mathcal{H})$ -valued functions  $E_j^\varepsilon$  and  $S_j^\varepsilon$  satisfy:*

$$\sum_{k=0}^{K+1-j} \|\partial_s^k E_j^\varepsilon(s)\| + \|\partial_s^k S_j^\varepsilon(s)\| = \tilde{\mathcal{O}}(\varepsilon^0), \quad E_j(s) \in \mathcal{L}(\mathcal{H}, D(A^\varepsilon(s))), \quad (\text{B.16})$$

$$A^\varepsilon(s)E_j(s) = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{and} \quad E_j(s)A^\varepsilon(s) = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{in } \mathcal{L}(\mathcal{H}), \quad (\text{B.17})$$

$$E_j^\varepsilon(s) = \sum_{m=0}^j E_m^\varepsilon(s)E_{j-m}^\varepsilon(s) \underset{\text{if } j \geq 1}{=} S_j^\varepsilon(s) + E_0^\varepsilon(s)E_j^\varepsilon(s) + E_j^\varepsilon(s)E_0^\varepsilon(s), \quad (\text{B.18})$$

$$i\partial_s E_{j-1}^\varepsilon(s) = [iA^\varepsilon(s), E_j^\varepsilon(s)], \quad \text{for } j \geq 1, \quad (\text{B.19})$$

with uniform constants w.r.t.  $s \in [0, T]$ .

**Proof:** The first statement for  $j = 0$  is a consequence of the definition (B.3) of  $E_0^\varepsilon(s) = P_0^\varepsilon(s)$  combined with the estimates (B.2) of  $\partial_s^k(z - iA^\varepsilon(s))^{-1}$ . By induction assume that the properties are satisfied for  $j \leq J < K$ . The definition (B.4) of  $S_{J+1}^\varepsilon$  and (B.5) of  $E_{J+1}^\varepsilon$  provide directly the first statement (B.16) for  $j = J + 1$ . The second statement of (B.16) and the estimates (B.17) rely on the bound of the  $\int_{\Gamma_\varepsilon}$ -term which is obtained after noticing

$$A^\varepsilon(s)R^\varepsilon = -1 + \frac{z}{(z - A^\varepsilon(s))} = R^\varepsilon A^\varepsilon(s) \quad (\text{B.20})$$

and the bound of the two other terms which is deduced from the induction assumption for  $j \leq J$ . Compute the commutator  $[iA^\varepsilon(s), S_{J+1}^\varepsilon(s)]$ :

$$\begin{aligned}
[iA^\varepsilon, S_{J+1}^\varepsilon] &= \sum_{m=1}^J (E_m^\varepsilon [iA^\varepsilon, E_{J+1-m}^\varepsilon] + [iA^\varepsilon, E_m^\varepsilon] E_{J+1-m}^\varepsilon), \\
&= \sum_{m=1}^J E_m^\varepsilon (i\partial_s E_{J-m}^\varepsilon) + (i\partial_s E_{m-1}^\varepsilon) E_{J+1-m}^\varepsilon, \quad \text{owing to (B.19) with } j \leq J, \\
&= i\partial_s E_J^\varepsilon - E_0^\varepsilon (i\partial_s E_J^\varepsilon) - (i\partial_s E_J^\varepsilon) E_0^\varepsilon, \quad \text{owing to (B.18) with } j \leq J, \\
&= -i(P_0^\varepsilon (\partial_s E_J^\varepsilon) P_0^\varepsilon - Q_0^\varepsilon (\partial_s E_J^\varepsilon) Q_0^\varepsilon), \quad \text{owing to } E_0^\varepsilon = P_0^\varepsilon = 1 - Q_0^\varepsilon.
\end{aligned}$$

With  $P_0^\varepsilon P_0^\varepsilon = P_0^\varepsilon$  and  $P_0^\varepsilon Q_0^\varepsilon = Q_0^\varepsilon P_0^\varepsilon = 0$ , this implies

$$[iA^\varepsilon, P_0^\varepsilon S_{J+1}^\varepsilon P_0^\varepsilon] = -iP_0^\varepsilon (\partial_s E_J^\varepsilon) P_0^\varepsilon, \quad (\text{B.21})$$

$$[iA^\varepsilon, Q_0^\varepsilon S_{J+1}^\varepsilon Q_0^\varepsilon] = iQ_0^\varepsilon (\partial_s E_J^\varepsilon) Q_0^\varepsilon, \quad (\text{B.22})$$

$$[iA^\varepsilon, P_0^\varepsilon S_{J+1}^\varepsilon Q_0^\varepsilon] = [iA^\varepsilon, Q_0^\varepsilon S_{J+1}^\varepsilon P_0^\varepsilon] = 0. \quad (\text{B.23})$$

The definition of  $P_0^\varepsilon$  as a spectral projection associated with  $iA^\varepsilon$  and (B.23), imply (see for example [43] Proposition 1)

$$P_0^\varepsilon S_{J+1}^\varepsilon Q_0^\varepsilon = Q_0^\varepsilon S_{J+1}^\varepsilon P_0^\varepsilon = 0.$$

Meanwhile the definition (B.5) of  $E_{J+1}^\varepsilon$  for  $j = J + 1$  implies

$$P_0^\varepsilon E_{J+1}^\varepsilon P_0^\varepsilon = -P_0^\varepsilon S_{J+1}^\varepsilon P_0^\varepsilon, \quad Q_0^\varepsilon E_{J+1}^\varepsilon Q_0^\varepsilon = Q_0^\varepsilon S_{J+1}^\varepsilon Q_0^\varepsilon.$$

This yields the relation (B.18) for  $j = J + 1$ . Another consequence with (B.21) and (B.22) is

$$[iA^\varepsilon, P_0^\varepsilon E_{J+1}^\varepsilon P_0^\varepsilon + Q_0^\varepsilon E_{J+1}^\varepsilon Q_0^\varepsilon] = P_0^\varepsilon (i\partial_s E_J^\varepsilon) P_0^\varepsilon + Q_0^\varepsilon (i\partial_s E_J^\varepsilon) Q_0^\varepsilon. \quad (\text{B.24})$$

Finally compute the off-diagonal blocks  $P_0^\varepsilon [iA^\varepsilon, E_{J+1}^\varepsilon] Q_0^\varepsilon$  and  $Q_0^\varepsilon [iA^\varepsilon, E_{J+1}^\varepsilon] P_0^\varepsilon$  by using again the definition (B.5) of  $E_{J+1}^\varepsilon$ , the relation (B.23), and the identity (B.20):

$$\begin{aligned}
[iA^\varepsilon, P_0^\varepsilon E_{J+1}^\varepsilon Q_0^\varepsilon] &= P_0^\varepsilon [iA^\varepsilon, E_{J+1}^\varepsilon] Q_0^\varepsilon = iP_0^\varepsilon (\partial_s E_J^\varepsilon) Q_0^\varepsilon, \\
[iA^\varepsilon, Q_0^\varepsilon E_{J+1}^\varepsilon P_0^\varepsilon] &= iQ_0^\varepsilon (\partial_s E_J^\varepsilon) P_0^\varepsilon.
\end{aligned}$$

Summing these last two equalities with (B.24) yields the relation (B.19) for  $j = J + 1$ .  $\square$   
The above calculations are essentially the same as in [43][44] and, as a consequence of Proposition B.3, the sum

$$T_\varepsilon(s) = \sum_{j=0}^K \varepsilon^j E_j^\varepsilon(s) \quad (\text{B.25})$$

solves (B.7), (B.9) and (B.10) in the sense of asymptotic expansions; in particular:

$$T_\varepsilon^2 = T_\varepsilon + \tilde{\mathcal{O}}(\varepsilon^{K+1}) \quad (\text{B.26})$$

Here comes the main difference which is necessary because no better estimate than  $\|P_0^\varepsilon\| = \tilde{\mathcal{O}}(\varepsilon^0)$  can be expected in our non self-adjoint case. We will need the next lemma.

**Lemma B.4.** *Assume that  $T \in \mathcal{L}(\mathcal{H})$  satisfies  $\|T^2 - T\| \leq \delta < 1/4$  and  $\|T\| \leq C$  then*

$$\begin{aligned}
\sigma(T) &\subset \{z \in \mathbb{C}, |z(z-1)| \leq \delta\} \subset \{z \in \mathbb{C}, |z| \leq c_\delta\} \cup \{z \in \mathbb{C}, |z-1| \leq c_\delta\}, \quad c_\delta < \frac{1}{2}, \\
\max \left\{ \|(z-T)^{-1}\|, |z-1| = \frac{1}{2} \right\} &\leq 2 \frac{2C+1}{1-4\delta}, \\
\|T-P\| &\leq 2 \frac{2C+1}{1-4\delta} \delta, \quad \text{with } P = \frac{1}{2i\pi} \int_{|z-1|=1/2} (z-T)^{-1} dz.
\end{aligned}$$

**Proof:** If  $z \in \sigma(T)$  then  $z(z-1)$  belongs to  $\sigma(T(T-1)) \subset \{z \in \mathbb{C}, |z(z-1)| \leq \frac{1}{4}\}$  (Remember that  $|z(z-1)| = \frac{1}{4}$  means  $|Z - \frac{1}{4}| = \frac{1}{4}$  with  $Z = (z - \frac{1}{2})^2$ ). Consider  $z \in \mathbb{C}$  such that  $|z-1| = \frac{1}{2}$ , then the relation

$$(T-z)(T-(1-z)) = z(1-z) + (T^2 - T),$$

with  $|z(1-z)| \geq \frac{1}{4}$  and  $\|T^2 - T\| \leq \delta < \frac{1}{4}$ , implies

$$\|(T-z)^{-1}\| \leq \|T - (1-z)\| \| [z(1-z) + T^2 - T]^{-1} \| \leq \frac{C + \frac{1}{2}}{\frac{1}{4} - \delta} \quad \text{for } |z-1| = \frac{1}{2}.$$

The symmetry with respect to  $z = \frac{1}{2}$  due to  $(1-T)(1-T) - (1-T) = T^2 - T$  implies also

$$\|(T-z)^{-1}\| \leq \frac{C + \frac{1}{2}}{\frac{1}{4} - \delta} \quad \text{for } |z| = \frac{1}{2}.$$

Compute

$$\begin{aligned} T - P &= \frac{1}{2i\pi} \int_{|z-1|=\frac{1}{2}} [T(z-1)^{-1} - (z-T)^{-1}] dz \\ &= (T-1)P + (T^2 - T)A_1 \quad \text{with} \quad A_1 = \frac{1}{2i\pi} \int_{|z-1|=\frac{1}{2}} (T-z)^{-1}(1-z)^{-1} dz. \end{aligned}$$

In particular this implies to  $T(1-P) = (T^2 - T)A_1$  while replacing  $T$  with  $(1-T)$  and  $P$  with  $1-P$  leads to

$$P - T = -T(1-P) + (T^2 - T)A_0 \quad \text{with} \quad A_0 = \frac{1}{2i\pi} \int_{|z|=\frac{1}{2}} (T-z)^{-1}z^{-1} dz.$$

We finally obtain

$$T - P = (T^2 - T)(A_1 - A_0) = (A_1 - A_0)(T^2 - T) \quad (\text{B.27})$$

$$\text{and} \quad \|T - P\| \leq \|T^2 - T\| [\|A_1\| + \|A_0\|] \leq \delta \times \frac{C + 1/2}{\frac{1}{4} - \delta}.$$

□

**Proposition B.5.** Consider the approximate projection  $T_\varepsilon(s)$  defined in (B.25), then there exists a projection  $P^\varepsilon(s)$  such that

$$\|P^\varepsilon(s) - T_\varepsilon(s)\| = \tilde{\mathcal{O}}(\varepsilon^{K+1}), \quad P^\varepsilon(s) \in \mathcal{L}(\mathcal{H}, D(A^\varepsilon(s))), \quad (\text{B.28})$$

$$\|A^\varepsilon(s)P^\varepsilon(s)\| = \tilde{\mathcal{O}}(\varepsilon^0) \quad \text{and} \quad \|P^\varepsilon(s)A^\varepsilon(s)\| = \tilde{\mathcal{O}}(\varepsilon^0), \quad (\text{B.29})$$

$$i\varepsilon\partial_s P^\varepsilon(s) = [iA^\varepsilon(s), P^\varepsilon(s)] + \tilde{\mathcal{O}}(\varepsilon^{K+1}), \quad \text{in } \mathcal{L}(\mathcal{H}). \quad (\text{B.30})$$

**Proof:** For  $\varepsilon > 0$  small enough, set

$$P^\varepsilon(s) = \frac{1}{2i\pi} \int_{|z-1|=\frac{1}{2}} (z - T_\varepsilon(s))^{-1} dz.$$

Owing to (B.26), the first statement of (B.28) is a straightforward application of Lemma B.4. The definition of  $T_\varepsilon(s)$  implies  $A^\varepsilon(s)T_\varepsilon(s) \in \mathcal{L}(\mathcal{H})$  and  $T_\varepsilon(s)A^\varepsilon(s) \in \mathcal{L}(\mathcal{H})$ . The relation (B.27) with  $T = T_\varepsilon$  and  $P = P^\varepsilon$  gives (B.29). Computing the derivative  $\partial_s P^\varepsilon(s)$  with  $T_\varepsilon \in \mathcal{C}^1([0, T]; \mathcal{L}(\mathcal{H}))$  gives:

$$\begin{aligned} i\varepsilon\partial_s P^\varepsilon &= \frac{1}{2i\pi} \int_{|z-1|=\frac{1}{2}} (z - T_\varepsilon)^{-1} (i\varepsilon\partial_s T_\varepsilon) (z - T_\varepsilon)^{-1} dz \\ &= \frac{1}{2i\pi} \int_{|z-1|=\frac{1}{2}} (z - T_\varepsilon)^{-1} [iA^\varepsilon, T_\varepsilon] (z - T_\varepsilon)^{-1} dz \\ &\quad + \frac{i\varepsilon^{K+1}}{2i\pi} \int_{|z-1|=\frac{1}{2}} (z - T_\varepsilon)^{-1} (\partial_s E_K^\varepsilon) (z - T_\varepsilon)^{-1} dz. \end{aligned}$$

The relation

$$[iA^\varepsilon, (z - T_\varepsilon)^{-1}] = (z - T_\varepsilon)^{-1} [iA^\varepsilon, T_\varepsilon] (z - T_\varepsilon)^{-1}$$

allows to conclude

$$i\varepsilon \partial_s P^\varepsilon - [iA^\varepsilon, P^\varepsilon] = \frac{i\varepsilon^{K+1}}{2i\pi} \int_{|z-1|=\frac{1}{2}} (z - T_\varepsilon)^{-1} (\partial_s E_K^\varepsilon) (z - T_\varepsilon)^{-1} dz = \tilde{\mathcal{O}}(\varepsilon^{K+1}).$$

□

**Proof of Theorem B.1:** The statements (B.7)(B.8) and (B.10) have already been checked in Proposition B.3 and Proposition B.5. Consider now the adiabatic evolution of  $S(t, s)u_s$ , when  $u_s = P^\varepsilon(s)u_s$ , stated in (B.11)(B.12)(B.13).

We assumed that the Cauchy problem (B.1) defines a strongly continuous dynamical system  $(S^\varepsilon(t, s))_{t \geq s \geq 0}$  of contractions in  $\mathcal{H}$  with  $S^\varepsilon(t, s)D(A^\varepsilon(s)) \subset D(A^\varepsilon(t))$ . We now consider the modified operator

$$\begin{aligned} H_{AD}^\varepsilon(t) &= iA^\varepsilon(t) + B^\varepsilon(t), \\ \text{with } B^\varepsilon(t) &= (1 - 2P^\varepsilon(t)) (i\varepsilon \partial_t P^\varepsilon(t) - [iA^\varepsilon(t), P^\varepsilon(t)]) . \end{aligned}$$

Since  $B^\varepsilon(s)$  is an  $\tilde{\mathcal{O}}(\varepsilon^{K+1})$  bounded continuous perturbation of  $iA^\varepsilon(s)$ , the Cauchy problem

$$\begin{cases} i\varepsilon \partial_t u_t = (iA^\varepsilon(t) - B^\varepsilon(t))u_t \\ u_{t=s} = u_s , \end{cases}$$

defines a strongly continuous dynamical system of bounded operators

$$S_{AD}^\varepsilon(t, s) = S^\varepsilon(t, s) - i\varepsilon^{-1} \int_s^t S^\varepsilon(t, s') (-B^\varepsilon(s')) S_{AD}^\varepsilon(s', s) ds' .$$

With the help of Gronwall lemma, it satisfies

$$\begin{aligned} \|S_{AD}^\varepsilon(t, s)\| &\leq e^{\varepsilon^{-1} \int_s^t \|B^\varepsilon(s')\| ds'} \leq e^{C_{\delta, T} \varepsilon^{K-\delta}(t-s)} \\ \|S^\varepsilon(t, s) - S_{AD}^\varepsilon(t, s)\| &\leq C_{\delta, T} \varepsilon^{K-\delta}(t-s) e^{C_{\delta, T} \varepsilon^{K-\delta}(t-s)} , \end{aligned}$$

for all  $s, t$ ,  $0 \leq s \leq t \leq T$ , with  $\delta \in (0, 1)$ . Note that the right-hand side is bounded when

$$K \geq 1 .$$

For the comparison (B.11) we take simply  $v^\varepsilon(t) = S_{AD}^\varepsilon(t, s)u_s$ . It remains to check (B.12) and (B.13). First notice the identity

$$\begin{aligned} H_{AD}^\varepsilon(t) &= P^\varepsilon(t)(iA^\varepsilon(t))P^\varepsilon(t) + (1 - P^\varepsilon(t))(iA^\varepsilon(t))(1 - P^\varepsilon(t)) \\ &\quad - i\varepsilon [P^\varepsilon(t)\partial_t P^\varepsilon(t) + (1 - P^\varepsilon(t))\partial_t(1 - P^\varepsilon(t))] . \end{aligned} \quad (\text{B.31})$$

For our choice  $v^\varepsilon(t) = S_{AD}^\varepsilon(t, s)u_s$  the quantity  $P^\varepsilon(t)(i\varepsilon \partial_t v^\varepsilon(t))$  equals  $P^\varepsilon(t)(iA^\varepsilon(t) + B^\varepsilon(t))v^\varepsilon(t)$  since  $P^\varepsilon(t)A^\varepsilon = A^\varepsilon(t)P^\varepsilon(t) - [A^\varepsilon(t), P^\varepsilon(t)] \in \mathcal{L}(\mathcal{H})$ . Hence  $P^\varepsilon(t)v^\varepsilon(t)$  satisfies in the strong sense the equation

$$\begin{aligned} (i\varepsilon \partial_t - H_{AD}^\varepsilon(t))(P^\varepsilon v^\varepsilon) &= i\varepsilon (\partial_t P^\varepsilon) v^\varepsilon + P^\varepsilon (H_{AD}^\varepsilon(t) v^\varepsilon) - H_{AD}^\varepsilon(t) P^\varepsilon(t) v^\varepsilon \\ &= i\varepsilon [(\partial_t P^\varepsilon) - P^\varepsilon (\partial_t P^\varepsilon) - (\partial_t P^\varepsilon) P^\varepsilon] v^\varepsilon(t) = 0 . \end{aligned}$$

As a strong solution to  $i\partial_t v = H_{AD}^\varepsilon(t)v(t)$  with the initial data  $P^\varepsilon(s)u_s = u_s$ ,  $P^\varepsilon(t)v^\varepsilon(t)$  has to be equal to  $v^\varepsilon(t)$ . We have proved (B.12). The equation (B.13) is a rewriting of  $i\varepsilon \partial_t v^\varepsilon - H_{AD}^\varepsilon(t)v^\varepsilon = 0$  after recalling  $\Pi(\partial\Pi)\Pi = 0$  when  $\Pi^2 = \Pi$ . □

**Proof of Corollary B.2:** Theorem B.1 applied with  $K = 1$  gives the approximation  $v^\varepsilon(t) = P^\varepsilon(t)v^\varepsilon(t)$ ,  $P^\varepsilon(t) = E_0^\varepsilon(t) + \varepsilon E_1^\varepsilon(t) + \tilde{\mathcal{O}}(\varepsilon^2)$ , which solves

$$\begin{cases} i\varepsilon \partial_t v^\varepsilon - i\varepsilon (\partial_t P^\varepsilon(t))v^\varepsilon = P^\varepsilon(t)(iA^\varepsilon(t))P^\varepsilon(t)v^\varepsilon , & \text{for } t \geq s , \\ v^\varepsilon(t = s) = u_s . \end{cases}$$

The relations  $P^\varepsilon = E_0^\varepsilon + \varepsilon E_1^\varepsilon + \tilde{\mathcal{O}}(\varepsilon^2)$ ,  $[A^\varepsilon, E_0^\varepsilon] = 0$  and  $E_0^\varepsilon E_1^\varepsilon E_0^\varepsilon = 0$  combined with the estimates (B.17) and (B.29) lead to:

$$P^\varepsilon(t)(iA^\varepsilon(t))P^\varepsilon(t) = E_0^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t) + \varepsilon E_1^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t) + \varepsilon(iA^\varepsilon(t))E_0^\varepsilon(t)E_1^\varepsilon(t) + \tilde{\mathcal{O}}(\varepsilon^2).$$

Then Proposition B.3 provide

$$i\varepsilon\partial_t P^\varepsilon(t) = i\varepsilon\partial_t E_0^\varepsilon(t) + \tilde{\mathcal{O}}(\varepsilon^2).$$

This implies

$$i\varepsilon\partial_t v^\varepsilon - i\varepsilon(\partial_t E_0^\varepsilon(t))v^\varepsilon = E_0^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t)v^\varepsilon + \varepsilon E_1^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t)v^\varepsilon + \tilde{\mathcal{O}}(\varepsilon^2), \quad (\text{B.32})$$

where we used  $E_0^\varepsilon v^\varepsilon = v^\varepsilon + \tilde{\mathcal{O}}(\varepsilon)$ . Consider now the adiabatic generator

$$\begin{aligned} H_0^\varepsilon(t) &= iA^\varepsilon(t) + B_0^\varepsilon(t), \\ \text{with } B_0^\varepsilon(t) &= (1 - 2E_0^\varepsilon(t))(i\varepsilon\partial_t E_0^\varepsilon(t) - [iA^\varepsilon(t), E_0^\varepsilon(t)]) = i\varepsilon(1 - 2E_0^\varepsilon(t))\partial_t E_0^\varepsilon(t). \end{aligned}$$

The assumed estimates on  $E_0$  and  $\partial_t E_0$  with the Gronwall Lemma lead to the uniform bound for the associated dynamical system  $S_0^\varepsilon(t, s)$ :

$$\forall s, t, 0 \leq s \leq t \leq T, \quad \|S_0^\varepsilon(t, s)\| \leq C_T e^{C_T},$$

while the formula (B.31) is valid for  $H_0^\varepsilon(t)$  after replacing  $P^\varepsilon(t)$  with  $E_0^\varepsilon(t)$ :

$$\begin{aligned} H_0^\varepsilon(t) &= E_0^\varepsilon(t)(iA^\varepsilon(t))E_0^\varepsilon(t) + (1 - E_0^\varepsilon(t))(iA^\varepsilon(t))(1 - E_0^\varepsilon(t)) \\ &\quad - i\varepsilon[E_0^\varepsilon(t)\partial_t E_0^\varepsilon(t) + (1 - E_0^\varepsilon(t))\partial_t(1 - E_0^\varepsilon(t))]. \end{aligned}$$

Now compute

$$(i\varepsilon\partial_t - H_0^\varepsilon(t))(E_0^\varepsilon v^\varepsilon) = i\varepsilon(\partial_t E_0^\varepsilon)v^\varepsilon + E_0^\varepsilon(i\varepsilon\partial_t v^\varepsilon) - H_0^\varepsilon(t)E_0(t)v^\varepsilon.$$

With (B.32) and  $E_0^\varepsilon E_1^\varepsilon E_0^\varepsilon = 0$ , one gets

$$(i\varepsilon\partial_t - H_0^\varepsilon(t))(E_0^\varepsilon v^\varepsilon) = -i\varepsilon[(\partial_t E_0^\varepsilon) - E_0^\varepsilon(\partial_t E_0^\varepsilon) - (\partial_t E_0^\varepsilon)E_0^\varepsilon]v^\varepsilon(t) + \tilde{\mathcal{O}}(\varepsilon^2) = \tilde{\mathcal{O}}(\varepsilon^2).$$

The uniform estimate  $\|S_0^\varepsilon(t, s)\| \leq C_T e^{C_T}$  implies

$$\|u^\varepsilon(t) - S_0^\varepsilon(t, s)u_s\| \leq \|u^\varepsilon(t) - v^\varepsilon(t)\| + \|\varepsilon E_1^\varepsilon(t)v^\varepsilon(t)\| + \|E_0^\varepsilon(t)v^\varepsilon - S_0^\varepsilon(t, s)u_s\| = \tilde{\mathcal{O}}(\varepsilon).$$

The same argument as in the end of the proof of Theorem B.1 says that  $v_0^\varepsilon(t) = S_0^\varepsilon(t, s)u_s$  with  $E_0^\varepsilon(s)u_s = u_s$  satisfies

$$\forall t \in [s, T], \quad E_0^\varepsilon(t)v_0^\varepsilon(t) = v_0^\varepsilon(t)$$

and solves the Cauchy problem

$$\begin{cases} i\varepsilon\partial_t v_0^\varepsilon - i\varepsilon(\partial_t E_0^\varepsilon(t))v_0^\varepsilon(t) = E_0^\varepsilon(t)(iA^\varepsilon(t))E_0(t)v_0^\varepsilon(t), \\ v_0^\varepsilon(t=s) = u_s. \end{cases}$$

The uniform boundedness of  $E_0^\varepsilon(t)$  and  $\partial_t E_0^\varepsilon(t)$  ensures that the solution to (B.14) is well defined for  $t', s' \in [0, T]$  with the uniform estimate

$$\forall t', s' \in [0, T], \quad \|\Phi_0^\varepsilon(t', s')\| \leq C'_T,$$

with the parallel transport property

$$\forall t', s' \in [0, T], \quad \Phi_0^\varepsilon(t', s')E_0^\varepsilon(s') = E_0^\varepsilon(t')\Phi_0^\varepsilon(t', s'), \quad [\Phi_0^\varepsilon(t', s')]^{-1} = \Phi_0^\varepsilon(s', t').$$

It suffices to take  $w^\varepsilon(t) = \Phi_0^\varepsilon(s, t)S_0^\varepsilon(t, s)u_s$ .  $\square$

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